

6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid

Other names:
acid

(R,S)-6-hydroxy-2,5,7,8-tetramethyl-2-chromancarboxylic acid

3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-carboxylic acid

Inchi: InChI=1S/C14H18O4/c1-7-8(2)12-10(9(3)11(7)15)5-6-14(4,18-12)13(16)17/h15H,5-6H2,

InchiKey: GLEVLJDDWXEYCO-UHFFFAOYSA-N

Formula: C14H18O4

SMILES: Cc1c(C)c2c(c(C)c1O)CCC(C)(C(=O)O)O2

Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	-322.43	kJ/mol	Joback Method
hf	-633.88	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
hvap	91.56	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.486		Crippen Method
mcvol	192.680	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	831.19	K	Joback Method
tc	1055.03	K	Joback Method
tf	463.00	K	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
vc	0.670	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.41	J/mol×K	831.19	Joback Method
cpg	599.12	J/mol×K	868.50	Joback Method

cpg	612.92	J/molxK	905.80	Joback Method
cpg	627.00	J/molxK	943.11	Joback Method
cpg	641.52	J/molxK	980.41	Joback Method
cpg	656.68	J/molxK	1017.72	Joback Method
cpg	672.64	J/molxK	1055.03	Joback Method
cps	368.90	J/molxK	338.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	335.10	J/molxK	303.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	338.40	J/molxK	308.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	342.00	J/molxK	313.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	349.80	J/molxK	318.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	353.50	J/molxK	323.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	363.00	J/molxK	328.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	332.00	J/molxK	298.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	372.10	J/molxK	343.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)

cps	375.10	J/mol×K	348.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	382.60	J/mol×K	353.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	387.90	J/mol×K	358.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	403.00	J/mol×K	368.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	408.40	J/mol×K	373.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	418.40	J/mol×K	378.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	427.70	J/mol×K	388.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	437.40	J/mol×K	393.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	448.30	J/mol×K	398.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
cps	453.30	J/mol×K	403.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)

cps	458.30	J/mol×K	408.15	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)
hvapt	133.80	kJ/mol	398.41	Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) and 6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of 2,2,5,7,8-pentamethylchroman-6-ol (PMC) Method:	https://www.doi.org/10.1016/j.jct.2013.11.032
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
6-hydroxy-2,5,7,8-tetramethylchroman-2-carboxylic acid (trolox) Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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