

«beta»-(4-Hydroxy-3-methoxyphenyl)propionic acid

Other names:
acid

3-(4-Hydroxy-3-methoxyphenyl)propionic acid

Benzenepropanoic acid, 4-hydroxy-3-methoxy-

Inchi:

InChI=1S/C10H12O4/c1-14-9-6-7(2-4-8(9)11)3-5-10(12)13/h2,4,6,11H,3,5H2,1H3,(H,12,

InchiKey:

BOLQJTPHPSDZHR-UHFFFAOYSA-N

Formula:

C10H12O4

SMILES:

COc1cc(CCC(=O)O)ccc1O

Mol. weight [g/mol]:

196.20

CAS:

1135-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-389.26	kJ/mol	Joback Method
hf	-599.01	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.418		Crippen Method
mvol	147.180	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	708.95	K	Joback Method
tc	917.59	K	Joback Method
tf	486.10	K	Joback Method
vc	0.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.98	J/mol×K	708.95	Joback Method
cpg	404.64	J/mol×K	743.72	Joback Method
cpg	413.76	J/mol×K	778.50	Joback Method
cpg	422.39	J/mol×K	813.27	Joback Method
cpg	430.57	J/mol×K	848.04	Joback Method
cpg	438.35	J/mol×K	882.82	Joback Method
cpg	445.79	J/mol×K	917.59	Joback Method

dvisc	0.0002007	Paxs	486.10	Joback Method
dvisc	0.0000856	Paxs	523.24	Joback Method
dvisc	0.0000409	Paxs	560.38	Joback Method
dvisc	0.0000214	Paxs	597.52	Joback Method
dvisc	0.0000121	Paxs	634.67	Joback Method
dvisc	0.0000073	Paxs	671.81	Joback Method
dvisc	0.0000046	Paxs	708.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1135235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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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