

1,3,5-Cyclohexanetriol, 2,2,4,4,6,6-hexamethyl-

Inchi:	InChI=1S/C12H24O3/c1-10(2)7(13)11(3,4)9(15)12(5,6)8(10)14/h7-9,13-15H,1-6H3
InchiKey:	SZRCMASKMMAGLQ-UHFFFAOYSA-N
Formula:	C12H24O3
SMILES:	CC1(C)C(O)C(C)(C)C(O)C(C)(C)C1O
Mol. weight [g/mol]:	216.32
CAS:	24413-59-0

Physical Properties

Property code	Value	Unit	Source
gf	-390.87	kJ/mol	Joback Method
hf	-749.36	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	87.77	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.161		Crippen Method
mcvol	186.690	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	747.42	K	Joback Method
tc	933.31	K	Joback Method
tf	465.34	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.15	J/molxK	747.42	Joback Method
cpg	615.22	J/molxK	778.40	Joback Method
cpg	630.35	J/molxK	809.38	Joback Method
cpg	645.72	J/molxK	840.36	Joback Method
cpg	661.48	J/molxK	871.35	Joback Method
cpg	677.80	J/molxK	902.33	Joback Method
cpg	694.85	J/molxK	933.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24413590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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