Cyclohexanepropanol, «alpha»,2,2,6-tetramethyl-

Other names: Tetrahydroionol
4-(2,2,6-Trimethylcyclohexyl)-2-butanol
«alpha»,2,2,6-tetramethylcyclohexanepropanol

Inchi: InChI=1S/C13H26O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h10-12,14H,5-9H2,1-4H3

InchiKey: UZWOWEPOVKVMEL-UHFFFAOYSA-N

Formula: C13H26O

SMILES: CC(O)CCC1C(C)CCCC1(C)C

Mol. weight [g/mol]: 198.34

CAS: 4361-23-3

Physical Properties

Property code	Value	Unit	Source
gf	-77.14	kJ/mol	Joback Method
hf	-440.28	kJ/mol	Joback Method
hfus	17.67	kJ/mol	Joback Method
hvap	59.48	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.610		Crippen Method
mcvol	189.040	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1432.80		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1424.00		NIST Webbook
tb	599.03	K	Joback Method
tc	788.62	K	Joback Method
tf	304.89	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.37	J/mol×K	599.03	Joback Method
cpg	541.27	J/mol×K	630.63	Joback Method
cpg	559.26	J/mol×K	662.23	Joback Method

cpg	576.42	J/mol×K	693.83	Joback Method
cpg	592.82	J/mol×K	725.43	Joback Method
cpg	608.54	J/mol×K	757.02	Joback Method
cpg	623.65	J/mol×K	788.62	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4361233&Units=SI

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume