1,3,3,5,5-Pentamethylcyclohexanol

Other names: Cyclohexanol, 1,3,3,5,5-pentamethyl-
Inchi: InChI=1S/C11H22O/c1-9(2)6-10(3,4)8-11(5,12)7-9/h12H,6-8H2,1-5H3
InchiKey: BMRINMQQUFUCHR-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CC1(C)CC(C)(C)CC(C)(O)C1
Mol. weight [g/mol]: 170.29
CAS: 38490-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-102.52	kJ/mol	Joback Method
hf	-363.24	kJ/mol	Joback Method
hfus	3.42	kJ/mol	Joback Method
hvap	53.12	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.974		Crippen Method
mcvol	160.860	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	554.19	K	Joback Method
tc	759.58	K	Joback Method
tf	345.15	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.07	J/mol×K	554.19	Joback Method
cpg	434.23	J/mol×K	588.42	Joback Method
cpg	450.34	J/mol×K	622.65	Joback Method
cpg	465.64	J/mol×K	656.88	Joback Method
cpg	480.35	J/mol×K	691.11	Joback Method
cpg	494.72	J/mol×K	725.35	Joback Method
cpg	508.98	J/mol×K	759.58	Joback Method

Sources

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=C38490334&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume