2-Cyclohexene-1-methanol, 2,6,6-trimethyl-

Other names: (2,6,6-Trimethyl-2-cyclohexen-1-yl)methanol
«alpha»-Cyclogeraniol
2,6,6-Trimethylcyclohex-2-ene-1-methanol
Inchi: InChI=1S/C10H18O/c1-8-5-4-6-10(2,3)9(8)7-11/h5,9,11H,4,6-7H2,1-3H3
InchiKey: WFBRXMMODZGJPF-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1=CCCC(C)(C)C1CO
Mol. weight [g/mol]: 154.25
CAS: 6627-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-71.92	kJ/mol	Joback Method
hf	-306.43	kJ/mol	Joback Method
hfus	13.18	kJ/mol	Joback Method
hvap	54.46	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.361		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1184.40		NIST Webbook
rinpol	1184.40		NIST Webbook
tb	539.64	K	Joback Method
tc	735.52	K	Joback Method
tf	303.60	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.85	J/mol×K	539.64	Joback Method
cpg	366.02	J/mol×K	572.29	Joback Method
cpg	380.37	J/mol×K	604.93	Joback Method
cpg	393.99	J/mol×K	637.58	Joback Method

cpg	406.95	J/mol×K	670.22	Joback Method
cpg	419.32	J/mol×K	702.87	Joback Method
cpg	431.19	J/mol×K	735.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6627743&Units=SI
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

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