2-Cyclohexen-1-ol, 2,6,6-trimethyl-

Other names: 2,6,6-Trimethyl-2-cyclohexen-1-ol
2,6,6-Trimethylcyclohex-2-enol
Inchi: InChI=1S/C9H16O/c1-7-5-4-6-9(2,3)8(7)10/h5,8,10H,4,6H2,1-3H3
InchiKey: QOIDDSNHBKJZNV-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC1=CCCC(C)(C)C1O
Mol. weight [g/mol]: 140.22
CAS: 54345-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-80.34	kJ/mol	Joback Method
hf	-285.79	kJ/mol	Joback Method
hfus	10.59	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.114		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1205.00		NIST Webbook
rinpol	1205.00		NIST Webbook
tb	516.76	K	Joback Method
tc	715.30	K	Joback Method
tf	292.33	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.39	J/mol×K	516.76	Joback Method
cpg	318.83	J/mol×K	549.85	Joback Method
cpg	332.45	J/mol×K	582.94	Joback Method
cpg	345.33	J/mol×K	616.03	Joback Method
cpg	357.55	J/mol×K	649.12	Joback Method

cpg	369.19	J/mol×K	682.21	Joback Method
cpg	380.33	J/mol×K	715.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54345594&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