1,3-Dimethylcyclopentanol

Inchi: InChI=1S/C7H14O/c1-6-3-4-7(2,8)5-6/h6,8H,3-5H2,1-2H3
InchiKey: LLIFEWZQIYEVKX-UHFFFAOYSA-N
Formula: C7H14O
SMILES: CC1CCC(C)(O)C1
Mol. weight [g/mol]: 114.19
CAS: 19550-46-0

Physical Properties

Property code	Value	Unit	Source
gf	-105.41	kJ/mol	Joback Method
hf	-284.66	kJ/mol	Joback Method
hfus	6.68	kJ/mol	Joback Method
hvap	46.65	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.557		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	462.59	K	Joback Method
tc	655.80	K	Joback Method
tf	254.55 ± 0.40	K	NIST Webbook
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.55	J/mol×K	462.59	Joback Method
cpg	246.05	J/mol×K	494.79	Joback Method
cpg	258.70	J/mol×K	526.99	Joback Method
cpg	270.57	J/mol×K	559.19	Joback Method
cpg	281.74	J/mol×K	591.40	Joback Method
cpg	292.30	J/mol×K	623.60	Joback Method
cpg	302.32	J/mol×K	655.80	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=C19550460&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume