3-Cyclohexene-1-methanol, «alpha»,4-dimethyl-

Other names: 1-(4-Methylcyclohex-3-en-1-yl)ethanol
Inchi: InChI=1S/C9H16O/c1-7-3-5-9(6-4-7)8(2)10/h3,8-10H,4-6H2,1-2H3
InchiKey: GLBZSENPZLIMDY-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC1=CCC(C(C)O)CC1
Mol. weight [g/mol]: 140.22
CAS: 55511-67-6

Physical Properties

Property code	Value	Unit	Source
gf	-69.58	kJ/mol	Joback Method
hf	-285.97	kJ/mol	Joback Method
hfus	12.30	kJ/mol	Joback Method
hvap	53.30	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.114		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1147.70		NIST Webbook
rinpol	1147.70		NIST Webbook
tb	520.75	K	Joback Method
tc	715.96	K	Joback Method
tf	257.67	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.77	J/mol×K	520.75	Joback Method
cpg	318.38	J/mol×K	553.28	Joback Method
cpg	332.26	J/mol×K	585.82	Joback Method
cpg	345.43	J/mol×K	618.35	Joback Method
cpg	357.92	J/mol×K	650.89	Joback Method
cpg	369.73	J/mol×K	683.42	Joback Method

cpg	380.88	J/mol×K	715.96	Joback Method
dvisc	0.0378551	Pa×s	257.67	Joback Method
dvisc	0.0073988	Pa×s	301.52	Joback Method
dvisc	0.0021888	Pa×s	345.36	Joback Method
dvisc	0.0008520	Pa×s	389.21	Joback Method
dvisc	0.0004015	Pa×s	433.06	Joback Method
dvisc	0.0002172	Pa×s	476.90	Joback Method
dvisc	0.0001304	Pa×s	520.75	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=C55511676&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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