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]: 140.23

Physical Properties

Property code	Value	Unit	Source
hf	-235.27	kJ/mol	Cheméo Relay (1.0)
hfus	12.30	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Cheméo Relay (1.0)
ie	8.65	eV	Cheméo Relay (1.0)
log10ws	-1.37		Cheméo Relay (1.0)
logp	2.114		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
rinpol	1147.70		NIST Webbook
rinpol	1147.70		NIST Webbook
tb	477.04	K	Cheméo Relay (1.0)
tf	294.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.77	J/mol×K	520.75	Joback Method
cpg	380.88	J/mol×K	715.96	Joback Method
cpg	369.73	J/mol×K	683.42	Joback Method
cpg	357.92	J/mol×K	650.89	Joback Method
cpg	345.43	J/mol×K	618.35	Joback Method
cpg	332.26	J/mol×K	585.82	Joback Method
cpg	318.38	J/mol×K	553.28	Joback Method
dvisc	0.0008520	Pa×s	389.21	Joback Method
dvisc	0.0001304	Pa×s	520.75	Joback Method
dvisc	0.0002172	Pa×s	476.90	Joback Method

dvisc	0.0004015	Pa×s	433.06	Joback Method
dvisc	0.0378551	Pa×s	257.67	Joback Method
dvisc	0.0021888	Pa×s	345.36	Joback Method
dvisc	0.0073988	Pa×s	301.52	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55511676&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point