6-Methyloctan-1-ol

Other names: 1-octanol, 6-methyl-
Inchi: InChI=1S/C9H20O/c1-3-9(2)7-5-4-6-8-10/h9-10H,3-8H2,1-2H3
InchiKey: WWRGKAMABZHMCN-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCC(C)CCCCCO
Mol. weight [g/mol]: 144.25
CAS: 38514-05-5

Physical Properties

Property code	Value	Unit	Source
gf	-114.36	kJ/mol	Joback Method
hf	-386.60	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.585		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1154.00		NIST Webbook
rinpol	1154.00		NIST Webbook
tb	479.15 ± 4.00	K	NIST Webbook
tc	659.14	K	Joback Method
tf	237.01	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.58	J/mol×K	497.06	Joback Method
cpg	347.30	J/mol×K	524.07	Joback Method
cpg	359.54	J/mol×K	551.09	Joback Method
cpg	371.30	J/mol×K	578.10	Joback Method
cpg	382.60	J/mol×K	605.11	Joback Method
cpg	393.45	J/mol×K	632.13	Joback Method

cpg	403.87	J/mol×K	659.14	Joback Method
dvisc	0.0878509	Pa×s	237.01	Joback Method
dvisc	0.0131188	Pa×s	280.35	Joback Method
dvisc	0.0032599	Pa×s	323.69	Joback Method
dvisc	0.0011254	Pa×s	367.03	Joback Method
dvisc	0.0004864	Pa×s	410.38	Joback Method
dvisc	0.0002468	Pa×s	453.72	Joback Method
dvisc	0.0001409	Pa×s	497.06	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C110453786&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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