

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:	WWRGKAMABZHM CN-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCC(C)CCCCO
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	m ³ /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	Paxs	237.01	Joback Method
dvisc	0.0131188	Paxs	280.35	Joback Method
dvisc	0.0032599	Paxs	323.69	Joback Method
dvisc	0.0011254	Paxs	367.03	Joback Method
dvisc	0.0004864	Paxs	410.38	Joback Method
dvisc	0.0002468	Paxs	453.72	Joback Method
dvisc	0.0001409	Paxs	497.06	Joback Method

Sources

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=C110453786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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