2-Hexyl-1-octanol

Other names: 1-Octanol, 2-hexyl-
Inchi: InChI=1S/C14H30O/c1-3-5-7-9-11-14(13-15)12-10-8-6-4-2/h14-15H,3-13H2,1-2H3
InchiKey: QNMCWJOEQBZQHB-UHFFFAOYSA-N
Formula: C14H30O
SMILES: CCCCCCC(CO)CCCCCC
Mol. weight [g/mol]: 214.39
CAS: 19780-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-72.26	kJ/mol	Joback Method
hf	-489.80	kJ/mol	Joback Method
hfus	32.58	kJ/mol	Joback Method
hvap	63.05	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.536		Crippen Method
mcvol	213.990	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
ripol	2069.00		NIST Webbook
ripol	2162.00		NIST Webbook
ripol	2162.00		NIST Webbook
ripol	2069.00		NIST Webbook
tb	611.46	K	Joback Method
tc	771.56	K	Joback Method
tf	293.36	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.00	J/mol×K	611.46	Joback Method
cpg	599.08	J/mol×K	638.14	Joback Method
cpg	614.51	J/mol×K	664.83	Joback Method
cpg	629.31	J/mol×K	691.51	Joback Method

cpg	643.50	J/mol×K	718.19	Joback Method
cpg	657.10	J/mol×K	744.87	Joback Method
cpg	670.12	J/mol×K	771.56	Joback Method
dvisc	0.0226239	Pa×s	293.36	Joback Method
dvisc	0.0038664	Pa×s	346.38	Joback Method
dvisc	0.0010562	Pa×s	399.39	Joback Method
dvisc	0.0003911	Pa×s	452.41	Joback Method
dvisc	0.0001784	Pa×s	505.43	Joback Method
dvisc	0.0000944	Pa×s	558.44	Joback Method
dvisc	0.0000558	Pa×s	611.46	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=C19780791&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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