1-Dodecanol, 2-methyl

Inchi: InChI=1S/C13H28O/c1-3-4-5-6-7-8-9-10-11-13(2)12-14/h13-14H,3-12H2,1-2H3
InchiKey: SCHAAFQMJJWGJM-UHFFFAOYSA-N
Formula: C13H28O
SMILES: CCCCCCCCCCC(C)CO
Mol. weight [g/mol]: 200.36
CAS: 22663-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-80.68	kJ/mol	Joback Method
hf	-469.16	kJ/mol	Joback Method
hfus	29.99	kJ/mol	Joback Method
hvap	60.82	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.146		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
tb	588.58	K	Joback Method
tc	748.59	K	Joback Method
tf	282.09	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.09	J/mol×K	588.58	Joback Method
cpg	601.64	J/mol×K	721.92	Joback Method
cpg	588.50	J/mol×K	695.25	Joback Method
cpg	574.79	J/mol×K	668.59	Joback Method
cpg	560.50	J/mol×K	641.92	Joback Method
cpg	545.60	J/mol×K	615.25	Joback Method
cpg	614.23	J/mol×K	748.59	Joback Method
dvisc	0.0000673	Pa×s	588.58	Joback Method
dvisc	0.0001145	Pa×s	537.50	Joback Method

dvisc	0.0002178	Pa×s	486.42	Joback Method
dvisc	0.0004818	Pa×s	435.33	Joback Method
dvisc	0.0013165	Pa×s	384.25	Joback Method
dvisc	0.0048963	Pa×s	333.17	Joback Method
dvisc	0.0293029	Pa×s	282.09	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=C22663612&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume