3-Methyldodecanol

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

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
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
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	545.60	J/mol×K	615.25	Joback Method
cpg	560.50	J/mol×K	641.92	Joback Method
cpg	574.79	J/mol×K	668.59	Joback Method
cpg	588.50	J/mol×K	695.25	Joback Method
cpg	601.64	J/mol×K	721.92	Joback Method
cpg	614.23	J/mol×K	748.59	Joback Method

dvisc	0.0293029	Pa×s	282.09	Joback Method
dvisc	0.0048963	Pa×s	333.17	Joback Method
dvisc	0.0013165	Pa×s	384.25	Joback Method
dvisc	0.0004818	Pa×s	435.33	Joback Method
dvisc	0.0002178	Pa×s	486.42	Joback Method
dvisc	0.0001145	Pa×s	537.50	Joback Method
dvisc	0.0000673	Pa×s	588.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56774e+01
Coeff. B	-4.99511e+03
Coeff. C	-8.95880e+01
Temperature range (K), min.	414.16
Temperature range (K), max.	571.46

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=R407917&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume