3-Methyltetradecanol

Inchi:	InChI=1S/C15H32O/c1-3-4-5-6-7-8-9-10-11-12-15(2)13-14-16/h15-16H,3-14H2,1-2H3
InchiKey:	MNHLRNCAHKCHDZ-UHFFFAOYSA-N
Formula:	C15H32O
SMILES:	CCCCCCCCCCCC(C)CCO
Mol. weight [g/mol]:	228.41
CAS:	---

Physical Properties

Property code	Value	Unit	Source
gf	-63.84	kJ/mol	Joback Method
hf	-510.44	kJ/mol	Joback Method
hfus	35.17	kJ/mol	Joback Method
hvap	65.27	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.926		Crippen Method
mcvol	228.080	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	1640.00		NIST Webbook
tb	634.34	K	Joback Method
tc	794.88	K	Joback Method
tf	304.63	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.33	J/mol×K	634.34	Joback Method
cpg	713.84	J/mol×K	768.12	Joback Method
cpg	699.82	J/mol×K	741.36	Joback Method
cpg	685.17	J/mol×K	714.61	Joback Method
cpg	669.89	J/mol×K	687.85	Joback Method
cpg	653.95	J/mol×K	661.10	Joback Method
cpg	727.26	J/mol×K	794.88	Joback Method
dvisc	0.0000463	Pa×s	634.34	Joback Method

dvisc	0.0000779	Pa×s	579.39	Joback Method
dvisc	0.0001462	Pa×s	524.44	Joback Method
dvisc	0.0003179	Pa×s	469.49	Joback Method
dvisc	0.0008492	Pa×s	414.53	Joback Method
dvisc	0.0030635	Pa×s	359.58	Joback Method
dvisc	0.0175571	Pa×s	304.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54497e+01
Coeff. B	-5.15231e+03
Coeff. C	-9.77060e+01
Temperature range (K), min.	437.52
Temperature range (K), max.	605.91

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407922&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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

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