2-Methyltetradecan-2-ol

Inchi: InChI=1S/C15H32O/c1-4-5-6-7-8-9-10-11-12-13-14-15(2,3)16/h16H,4-14H2,1-3H3
InchiKey: IBIINSQLHLWOMP-UHFFFAOYSA-N
Formula: C15H32O
SMILES: CCCCCCCCCCCCC(C)(C)O
Mol. weight [g/mol]: 228.42

Physical Properties

Property code	Value	Unit	Source
af	0.8888		Cheméo Relay (1.0)
gf	-58.56	kJ/mol	Joback Method
hf	-548.44	kJ/mol	Cheméo Relay (1.0)
hfus	31.28	kJ/mol	Joback Method
hvap	94.16	kJ/mol	Cheméo Relay (1.0)
ie	9.83	eV	Cheméo Relay (1.0)
log10ws	-5.57		Cheméo Relay (1.0)
logp	5.068		Crippen Method
mcvol	228.080	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1630.80		NIST Webbook
rinpol	1630.80		NIST Webbook
tb	554.64	K	Cheméo Relay (1.0)
tc	724.63	K	Cheméo Relay (1.0)
tf	309.52	K	Cheméo Relay (1.0)
vc	0.892	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.49	J/mol×K	631.55	Joback Method
cpg	656.34	J/mol×K	658.88	Joback Method
cpg	672.44	J/mol×K	686.22	Joback Method
cpg	687.82	J/mol×K	713.55	Joback Method
cpg	702.51	J/mol×K	740.88	Joback Method
cpg	716.54	J/mol×K	768.22	Joback Method

cpg	729.95	J/mol×K	795.55	Joback Method
dvisc	0.0119050	Pa×s	322.05	Joback Method
dvisc	0.0024550	Pa×s	373.63	Joback Method
dvisc	0.0007426	Pa×s	425.22	Joback Method
dvisc	0.0002909	Pa×s	476.80	Joback Method
dvisc	0.0001369	Pa×s	528.38	Joback Method
dvisc	0.0000736	Pa×s	579.97	Joback Method
dvisc	0.0000438	Pa×s	631.55	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27570838&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie: Ionization energy
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