2-PENTADECANOL

Other names:	Pentadecan-2-ol
	sec-Pentadecyl alcohol
Inchi:	InChI=1S/C15H32O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15(2)16/h15-16H,3-14H2,1-2H3
InchiKey:	ALVGHPMGQNBJRC-UHFFFAOYSA-N
Formula:	C15H32O
SMILES:	CCCCCCCCCCCCCC(C)O
Mol. weight [g/mol]:	228.42
CAS:	1653-34-5

Physical Properties

Property code	Value	Unit	Source
af	0.8941		Cheméo Relay (1.0)
gf	-63.84	kJ/mol	Joback Method
hf	-540.55	kJ/mol	Cheméo Relay (1.0)
hfus	35.17	kJ/mol	Joback Method
hvap	101.36	kJ/mol	Cheméo Relay (1.0)
ie	9.88	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	1528.27	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1690.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2128.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2092.00		NIST Webbook
tb	564.66	K	Cheméo Relay (1.0)
tc	732.83	K	Cheméo Relay (1.0)
tf	314.22	K	Cheméo Relay (1.0)
vc	0.903	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.33	J/mol×K	634.34	Joback Method
cpg	653.95	J/mol×K	661.10	Joback Method
cpg	669.89	J/mol×K	687.85	Joback Method
cpg	685.17	J/mol×K	714.61	Joback Method
cpg	699.82	J/mol×K	741.36	Joback Method
cpg	713.84	J/mol×K	768.12	Joback Method
cpg	727.26	J/mol×K	794.88	Joback Method
dvisc	0.0175571	Pa×s	304.63	Joback Method
dvisc	0.0030635	Pa×s	359.58	Joback Method
dvisc	0.0008492	Pa×s	414.53	Joback Method
dvisc	0.0003179	Pa×s	469.49	Joback Method
dvisc	0.0001462	Pa×s	524.44	Joback Method
dvisc	0.0000779	Pa×s	579.39	Joback Method
dvisc	0.0000463	Pa×s	634.34	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

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1653345&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

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