

1,14-Tetradecanediol

Other names:	tetradecamethylene glycol tetradecane-1,14-diol
Inchi:	InChI=1S/C14H30O2/c15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16/h15-16H,1-14H2
InchiKey:	XLKZJJVNBQCVIX-UHFFFAOYSA-N
Formula:	C14H30O2
SMILES:	OCCCCCCCCCCCCCO
Mol. weight [g/mol]:	230.39
CAS:	19812-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-206.64	kJ/mol	Joback Method
hf	-636.75	kJ/mol	Joback Method
hfus	40.19	kJ/mol	Joback Method
hvap	80.12	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.652		Crippen Method
mcvol	219.860	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1924.00		NIST Webbook
tb	704.08	K	Joback Method
tc	867.15	K	Joback Method
tf	359.20	K	Thermodynamics of fusion and sublimation for a homologous series of eleven alkane-.alpha.,.omega.-diols HO-(CH2)n-OH: Structure-related odd even effect
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.47	J/mol×K	839.97	Joback Method

cpg	706.50	J/mol×K	812.79	Joback Method
cpg	693.98	J/mol×K	785.61	Joback Method
cpg	680.89	J/mol×K	758.44	Joback Method
cpg	667.21	J/mol×K	731.26	Joback Method
cpg	652.92	J/mol×K	704.08	Joback Method
cpg	729.92	J/mol×K	867.15	Joback Method
dvisc	0.0071914	Pa×s	369.18	Joback Method
dvisc	0.0000105	Pa×s	704.08	Joback Method
dvisc	0.0000195	Pa×s	648.26	Joback Method
dvisc	0.0000407	Pa×s	592.45	Joback Method
dvisc	0.0000992	Pa×s	536.63	Joback Method
dvisc	0.0002969	Pa×s	480.81	Joback Method
dvisc	0.0011853	Pa×s	425.00	Joback Method
hfust	61.90	kJ/mol	360.40	NIST Webbook
hvapt	149.70	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.49574e+01
Coeff. B	-9.22020e+03
Coeff. C	-1.15776e+02
Temperature range (K), min.	489.52
Temperature range (K), max.	585.09

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

Thermodynamics of fusion and sublimation for a homologous series of r,o-Alkanediols by Correlation Gas Chromatography:
Joback Method:

<https://www.doi.org/10.1016/j.jct.2013.08.019>

<https://www.doi.org/10.1021/je060333x>

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=C19812647&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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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