Tetradecanedioic acid

Other names:	1,12-Dodecanedicarboxylic acid
	1,14-Tetradecanedioic acid
	Dodecamethylenedicarboxylic acid
	Tetradecane-1,14-dioic acid
	Tetradecanedicarboxylic acid
Inchi:	InChI=1S/C14H26O4/c15-13(16)11-9-7-5-3-1-2-4-6-8-10-12-14(17)18/h1-12H2,(H,15,16)
InchiKey:	HQHCYKULIHKCEB-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	O=C(O)CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	258.35
CAS:	821-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-464.48	kJ/mol	Joback Method
hf	-861.91	kJ/mol	Joback Method
hfus	56.50	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hvap	127.40 ± 2.30	kJ/mol	NIST Webbook
log10ws	-3.88		Crippen Method
logp	3.837		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1900.00	kPa	Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14)
tb	811.82	K	Joback Method
tc	995.10	K	Joback Method
tf	469.04	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	690.30	J/mol×K	811.82	Joback Method
cpg	702.78	J/mol×K	842.37	Joback Method
cpg	714.59	J/mol×K	872.91	Joback Method
cpg	725.74	J/mol×K	903.46	Joback Method
cpg	736.26	J/mol×K	934.01	Joback Method
cpg	746.18	J/mol×K	964.56	Joback Method
cpg	755.53	J/mol×K	995.10	Joback Method
dvisc	0.0009163	Pa×s	469.04	Joback Method
dvisc	0.0002530	Pa×s	526.17	Joback Method
dvisc	0.0000899	Pa×s	583.30	Joback Method
dvisc	0.0000384	Pa×s	640.43	Joback Method
dvisc	0.0000189	Pa×s	697.56	Joback Method
dvisc	0.0000103	Pa×s	754.69	Joback Method
dvisc	0.0000061	Pa×s	811.82	Joback Method
hfust	56.50	kJ/mol	397.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50708e+01
Coeff. B	-5.98314e+03
Coeff. C	-1.28547e+02
Temperature range (K), min.	533.27
Temperature range (K), max.	741.61

Sources

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=C821385&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
Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16:	https://www.doi.org/10.1016/j.jct.2004.12.011
Critical Temperatures and Pressures of Straight-Chain Saturated Dicarboxylic Acids (C4 to C14):	https://www.doi.org/10.1021/je0498356

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume