

15-Hydroxypentadecanoic acid

Other names:	Pentadecanoic acid, 15-hydroxy-
Inchi:	InChI=1S/C15H30O3/c16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15(17)18/h16H,1-14H2,(H,1
InchiKey:	BZUNJUAMQZRJIP-UHFFFAOYSA-N
Formula:	C15H30O3
SMILES:	O=C(O)CCCCCCCCCCCCCO
Mol. weight [g/mol]:	258.40
CAS:	4617-33-8

Physical Properties

Property code	Value	Unit	Source
gf	-327.14	kJ/mol	Joback Method
hf	-769.97	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	89.09	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.135		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
tb	780.83	K	Joback Method
tc	957.13	K	Joback Method
tf	430.38	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.68	J/molxK	957.13	Joback Method
cpg	793.80	J/molxK	927.75	Joback Method
cpg	782.34	J/molxK	898.37	Joback Method
cpg	770.26	J/molxK	868.98	Joback Method
cpg	757.54	J/molxK	839.60	Joback Method
cpg	744.16	J/molxK	810.21	Joback Method
cpg	730.08	J/molxK	780.83	Joback Method
dvisc	0.0017796	Paxs	430.38	Joback Method

dvisc	0.0000063	Paxs	780.83	Joback Method
dvisc	0.0000111	Paxs	722.42	Joback Method
dvisc	0.0000214	Paxs	664.01	Joback Method
dvisc	0.0000469	Paxs	605.61	Joback Method
dvisc	0.0001217	Paxs	547.20	Joback Method
dvisc	0.0003965	Paxs	488.79	Joback Method
hsubt	103.00	kJ/mol	305.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4617338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hsubt:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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