

3-Hydroxyhexadecane-1-sulfonic acid, gamma-sultone

Inchi:	InChI=1S/C16H32O3S/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-14-15-20(17,18)19-16/h16H,2
InchiKey:	UEBQFXPPZASWJO-UHFFFAOYSA-N
Formula:	C16H32O3S
SMILES:	CCCCCCCCCCCCC1CCS(=O)(=O)O1
Mol. weight [g/mol]:	304.49
CAS:	1633-76-7

Physical Properties

Property code	Value	Unit	Source
gf	-427.53	kJ/mol	Joback Method
hf	-895.05	kJ/mol	Joback Method
hfus	50.01	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.806		Crippen Method
mvol	259.400	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
tb	634.54	K	Joback Method
tc	805.04	K	Joback Method
tf	395.16	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.18	J/mol×K	634.54	Joback Method
cpg	746.08	J/mol×K	662.96	Joback Method
cpg	765.03	J/mol×K	691.37	Joback Method
cpg	783.06	J/mol×K	719.79	Joback Method
cpg	800.19	J/mol×K	748.21	Joback Method
cpg	816.44	J/mol×K	776.62	Joback Method
cpg	831.84	J/mol×K	805.04	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1633767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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