1,2-Oxathiane, 6-dodecyl-, 2,2-dioxide

Other names: «delta»-Hexadecanesultone
Hexadecyl 1,4-sultone
Hexadecane-1-sulfonic acid, 4-hydroxy-, delta-sultone
Inchi: InChI=1S/C16H32O3S/c1-2-3-4-5-6-7-8-9-10-11-13-16-14-12-15-20(17,18)19-16/h16H,2
InchiKey: QPGWMTLYKYBJSB-UHFFFAOYSA-N
Formula: C16H32O3S
SMILES: CCCCCCCCCCCCC1CCCS(=O)(=O)O1
Mol. weight [g/mol]: 304.49
CAS: 15224-88-1

Physical Properties

Property code	Value	Unit	Source
gf	-439.63	kJ/mol	Joback Method
hf	-901.21	kJ/mol	Joback Method
hfus	47.91	kJ/mol	Joback Method
hvap	73.78	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.806		Crippen Method
mcvol	259.400	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
tb	638.81	K	Joback Method
tc	813.64	K	Joback Method
tf	391.64	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.12	J/mol×K	638.81	Joback Method
cpg	749.74	J/mol×K	667.95	Joback Method
cpg	769.34	J/mol×K	697.09	Joback Method
cpg	787.95	J/mol×K	726.23	Joback Method
cpg	805.58	J/mol×K	755.37	Joback Method
cpg	822.26	J/mol×K	784.50	Joback Method

cpg	838.02	J/mol×K	813.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15224881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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