Pentadecyl sulfuric acid

Inchi: InChI=1S/C15H32O4S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-20(16,17)18/h2-15H2,1
InchiKey: COUMKTRLCGRAAA-UHFFFAOYSA-N
Formula: C15H32O4S
SMILES: CCCCCCCCCCCCCCCOS(=O)(=O)O
Mol. weight [g/mol]: 308.48
CAS: 45247-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-634.94	kJ/mol	Joback Method
hf	-1090.73	kJ/mol	Joback Method
hfl	-1175.00 ± 8.00	kJ/mol	NIST Webbook
hfus	51.26	kJ/mol	Joback Method
hvap	86.71	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.897		Crippen Method
mcvol	262.040	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
tb	704.98	K	Joback Method
tc	868.67	K	Joback Method
tf	380.42	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.32	J/mol×K	704.98	Joback Method
cpg	779.58	J/mol×K	732.26	Joback Method
cpg	795.08	J/mol×K	759.54	Joback Method
cpg	809.82	J/mol×K	786.82	Joback Method
cpg	823.81	J/mol×K	814.11	Joback Method
cpg	837.05	J/mol×K	841.39	Joback Method
cpg	849.55	J/mol×K	868.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C45247345&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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