

Octadecane-1-sulfonic acid, 4-hydroxy-, delta-sultone

Inchi:	InChI=1S/C18H36O3S/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-16-14-17-22(19,20)21-18/H
InchiKey:	YWXGDDUJIRWXGV-UHFFFAOYSA-N
Formula:	C18H36O3S
SMILES:	CCCCCCCCCCCCCCCC1CCCS(=O)(=O)O1
Mol. weight [g/mol]:	332.54
CAS:	29638-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-422.79	kJ/mol	Joback Method
hf	-942.49	kJ/mol	Joback Method
hfus	53.09	kJ/mol	Joback Method
hvap	78.23	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.586		Crippen Method
mcvol	287.580	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
tb	684.57	K	Joback Method
tc	858.77	K	Joback Method
tf	414.18	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.94	J/molxK	684.57	Joback Method
cpg	867.02	J/molxK	713.60	Joback Method
cpg	887.02	J/molxK	742.64	Joback Method
cpg	905.98	J/molxK	771.67	Joback Method
cpg	923.91	J/molxK	800.70	Joback Method
cpg	940.85	J/molxK	829.74	Joback Method
cpg	956.82	J/molxK	858.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29638662&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	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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