

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

Inchi:	InChI=1S/C14H28O3S/c1-2-3-4-5-6-7-8-9-11-14-12-10-13-18(15,16)17-14/h14H,2-13H2
InchiKey:	FPGWFFVPBMXANA-UHFFFAOYSA-N
Formula:	C14H28O3S
SMILES:	CCCCCCCCCCC1CCCS(=O)(=O)O1
Mol. weight [g/mol]:	276.44
CAS:	40146-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-456.47	kJ/mol	Joback Method
hf	-859.93	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.026		Crippen Method
mvol	231.220	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
tb	593.05	K	Joback Method
tc	769.96	K	Joback Method
tf	369.10	K	Joback Method
vc	0.891	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.06	J/mol×K	593.05	Joback Method
cpg	637.11	J/mol×K	622.53	Joback Method
cpg	656.18	J/mol×K	652.02	Joback Method
cpg	674.31	J/mol×K	681.50	Joback Method
cpg	691.51	J/mol×K	710.99	Joback Method
cpg	707.81	J/mol×K	740.47	Joback Method
cpg	723.21	J/mol×K	769.96	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40146870&Units=SI

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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