Methanesulfonamide, N,N-dioctyl-

Inchi: InChI=1S/C17H37NO2S/c1-4-6-8-10-12-14-16-18(21(3,19)20)17-15-13-11-9-7-5-2/h4-17
InchiKey: XHHHTXDICJDRSR-UHFFFAOYSA-N
Formula: C17H37NO2S
SMILES: CCCCCCCCN(CCCCCCCC)S(C)(=O)=O
Mol. weight [g/mol]: 319.55

Physical Properties

Property code	Value	Unit	Source
gf	-265.50	kJ/mol	Joback Method
hf	-780.03	kJ/mol	Joback Method
hfus	54.18	kJ/mol	Joback Method
hvap	74.11	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.969		Crippen Method
mcvol	288.460	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	2263.00		NIST Webbook
rinpol	2263.00		NIST Webbook
tb	648.58	K	Joback Method
tc	807.86	K	Joback Method
tf	352.38	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.41	J/mol×K	648.58	Joback Method
cpg	828.02	J/mol×K	675.13	Joback Method
cpg	846.76	J/mol×K	701.67	Joback Method
cpg	864.67	J/mol×K	728.22	Joback Method
cpg	881.74	J/mol×K	754.77	Joback Method
cpg	898.00	J/mol×K	781.32	Joback Method
cpg	913.48	J/mol×K	807.86	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=U308434&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume