Methylsulphonamide, N-ethyl-N-octadecyl-

Inchi: InChI=1S/C21H45NO2S/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(5-2)25(3
InchiKey: LDCFEXYKHVLWFJ-UHFFFAOYSA-N
Formula: C21H45NO2S
SMILES: CCCCCCCCCCCCCCCCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 375.65

Physical Properties

Property code	Value	Unit	Source
gf	-231.82	kJ/mol	Joback Method
hf	-862.59	kJ/mol	Joback Method
hfus	64.55	kJ/mol	Joback Method
hvap	83.02	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.529		Crippen Method
mcvol	344.820	ml/mol	McGowan Method
pc	1053.46	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	740.10	K	Joback Method
tc	908.11	K	Joback Method
tf	397.46	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.11	J/mol×K	740.10	Joback Method
cpg	1071.44	J/mol×K	768.10	Joback Method
cpg	1091.71	J/mol×K	796.10	Joback Method
cpg	1110.95	J/mol×K	824.10	Joback Method
cpg	1129.18	J/mol×K	852.11	Joback Method
cpg	1146.44	J/mol×K	880.11	Joback Method
cpg	1162.76	J/mol×K	908.11	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=U415447&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