Methylsulphonamide, N-ethyl-N-hexadecyl-

Inchi: InChI=1S/C19H41NO2S/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(5-2)23(3,21)22
InchiKey: SSDRRENMOQEGSU-UHFFFAOYSA-N
Formula: C19H41NO2S
SMILES: CCCCCCCCCCCCCCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 347.60

Physical Properties

Property code	Value	Unit	Source
gf	-248.66	kJ/mol	Joback Method
hf	-821.31	kJ/mol	Joback Method
hfus	59.36	kJ/mol	Joback Method
hvap	78.57	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.749		Crippen Method
mcvol	316.640	ml/mol	McGowan Method
pc	1198.13	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	694.34	K	Joback Method
tc	856.85	K	Joback Method
tf	374.92	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.29	J/mol×K	694.34	Joback Method
cpg	947.73	J/mol×K	721.42	Joback Method
cpg	967.21	J/mol×K	748.51	Joback Method
cpg	985.77	J/mol×K	775.59	Joback Method
cpg	1003.42	J/mol×K	802.68	Joback Method
cpg	1020.19	J/mol×K	829.76	Joback Method
cpg	1036.10	J/mol×K	856.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415446&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

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