Methylsulphonamide, N-ethyl-N-octyl-

Inchi: InChI=1S/C11H25NO2S/c1-4-6-7-8-9-10-11-12(5-2)15(3,13)14/h4-11H2,1-3H3
InchiKey: MMZUDBJPQUGONP-UHFFFAOYSA-N
Formula: C11H25NO2S
SMILES: CCCCCCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 235.39

Physical Properties

Property code	Value	Unit	Source
gf	-316.02	kJ/mol	Joback Method
hf	-656.19	kJ/mol	Joback Method
hfus	38.64	kJ/mol	Joback Method
hvap	60.76	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.628		Crippen Method
mcvol	203.920	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	511.30	K	Joback Method
tc	669.97	K	Joback Method
tf	284.76	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.29	J/mol×K	511.30	Joback Method
cpg	499.00	J/mol×K	537.75	Joback Method
cpg	515.05	J/mol×K	564.19	Joback Method
cpg	530.45	J/mol×K	590.64	Joback Method
cpg	545.22	J/mol×K	617.08	Joback Method
cpg	559.36	J/mol×K	643.53	Joback Method
cpg	572.88	J/mol×K	669.97	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415440&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
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