Methylsulphonamide, N-ethyl-N-hexyl-

Inchi: InChI=1S/C9H21NO2S/c1-4-6-7-8-9-10(5-2)13(3,11)12/h4-9H2,1-3H3
InchiKey: ZJINUAVGCLHLEA-UHFFFAOYSA-N
Formula: C9H21NO2S
SMILES: CCCCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 207.33

Physical Properties

Property code	Value	Unit	Source
gf	-332.86	kJ/mol	Joback Method
hf	-614.91	kJ/mol	Joback Method
hfus	33.46	kJ/mol	Joback Method
hvap	56.31	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.848		Crippen Method
mcvol	175.740	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
tb	465.54	K	Joback Method
tc	625.53	K	Joback Method
tf	262.22	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.34	J/mol×K	465.54	Joback Method
cpg	401.63	J/mol×K	492.21	Joback Method
cpg	416.34	J/mol×K	518.87	Joback Method
cpg	430.48	J/mol×K	545.54	Joback Method
cpg	444.05	J/mol×K	572.20	Joback Method
cpg	457.06	J/mol×K	598.87	Joback Method
cpg	469.52	J/mol×K	625.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415437&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