Methylsulphonamide, N-ethyl-N-propyl-

Inchi: InChI=1S/C6H15NO2S/c1-4-6-7(5-2)10(3,8)9/h4-6H2,1-3H3
InchiKey: QLFWVEHQNOBTCP-UHFFFAOYSA-N
Formula: C6H15NO2S
SMILES: CCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 165.25

Physical Properties

Property code	Value	Unit	Source
gf	-358.12	kJ/mol	Joback Method
hf	-552.99	kJ/mol	Joback Method
hfus	25.70	kJ/mol	Joback Method
hvap	49.63	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	0.678		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	396.90	K	Joback Method
tc	558.65	K	Joback Method
tf	228.41	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.33	J/mol×K	396.90	Joback Method
cpg	269.78	J/mol×K	423.86	Joback Method
cpg	281.79	J/mol×K	450.82	Joback Method
cpg	293.35	J/mol×K	477.77	Joback Method
cpg	304.48	J/mol×K	504.73	Joback Method
cpg	315.18	J/mol×K	531.69	Joback Method
cpg	325.44	J/mol×K	558.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415432&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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