Methylsulphonamide, N-ethyl-N-pentyl-

Inchi: InChI=1S/C8H19NO2S/c1-4-6-7-8-9(5-2)12(3,10)11/h4-8H2,1-3H3
InchiKey: LYAJICLUKDATIT-UHFFFAOYSA-N
Formula: C8H19NO2S
SMILES: CCCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 193.31

Physical Properties

Property code	Value	Unit	Source
gf	-341.28	kJ/mol	Joback Method
hf	-594.27	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	54.08	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	1.458		Crippen Method
mcvol	161.650	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1739.00		NIST Webbook
rinpol	1739.00		NIST Webbook
tb	442.66	K	Joback Method
tc	603.33	K	Joback Method
tf	250.95	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.24	J/mol×K	442.66	Joback Method
cpg	355.68	J/mol×K	469.44	Joback Method
cpg	369.59	J/mol×K	496.22	Joback Method
cpg	382.97	J/mol×K	523.00	Joback Method
cpg	395.82	J/mol×K	549.78	Joback Method
cpg	408.15	J/mol×K	576.56	Joback Method
cpg	419.97	J/mol×K	603.33	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=U415436&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