

Methylsulphonamide, N-ethyl-N-2-ethylhexyl-

Inchi:	InChI=1S/C11H25NO2S/c1-5-8-9-11(6-2)10-12(7-3)15(4,13)14/h11H,5-10H2,1-4H3
InchiKey:	NUOQSHFZRDDUPY-UHFFFAOYSA-N
Formula:	C11H25NO2S
SMILES:	CCCCC(CC)CN(CC)S(C)(=O)=O
Mol. weight [g/mol]:	235.39

Physical Properties

Property code	Value	Unit	Source
gf	-318.46	kJ/mol	Joback Method
hf	-661.47	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.484		Crippen Method
mvol	203.920	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	510.86	K	Joback Method
tc	672.42	K	Joback Method
tf	269.76	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.45	J/molxK	510.86	Joback Method
cpg	499.52	J/molxK	537.79	Joback Method
cpg	515.91	J/molxK	564.71	Joback Method
cpg	531.62	J/molxK	591.64	Joback Method
cpg	546.67	J/molxK	618.57	Joback Method
cpg	561.06	J/molxK	645.49	Joback Method
cpg	574.81	J/molxK	672.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415438&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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