

Methylsulphonamide, N-ethyl-N-dodecyl-

Inchi:	InChI=1S/C15H33NO2S/c1-4-6-7-8-9-10-11-12-13-14-15-16(5-2)19(3,17)18/h4-15H2,1-3
InchiKey:	JQPPVBIFGQDXHC-UHFFFAOYSA-N
Formula:	C15H33NO2S
SMILES:	CCCCCCCCCCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]:	291.49

Physical Properties

Property code	Value	Unit	Source
gf	-282.34	kJ/mol	Joback Method
hf	-738.75	kJ/mol	Joback Method
hfus	49.00	kJ/mol	Joback Method
hvap	69.66	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.189		Crippen Method
mcvol	260.280	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	602.82	K	Joback Method
tc	760.68	K	Joback Method
tf	329.84	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.12	J/mol×K	602.82	Joback Method
cpg	712.90	J/mol×K	629.13	Joback Method
cpg	730.88	J/mol×K	655.44	Joback Method
cpg	748.09	J/mol×K	681.75	Joback Method
cpg	764.53	J/mol×K	708.06	Joback Method
cpg	780.23	J/mol×K	734.37	Joback Method
cpg	795.20	J/mol×K	760.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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