Methylsulphonamide, N-ethyl-N-nonyl-

Inchi: InChI=1S/C12H27NO2S/c1-4-6-7-8-9-10-11-12-13(5-2)16(3,14)15/h4-12H2,1-3H3
InchiKey: VVBKVSIUOPYGQW-UHFFFAOYSA-N
Formula: C12H27NO2S
SMILES: CCCCCCCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 249.41

Physical Properties

Property code	Value	Unit	Source
gf	-307.60	kJ/mol	Joback Method
hf	-676.83	kJ/mol	Joback Method
hfus	41.23	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.018		Crippen Method
mcvol	218.010	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
tb	534.18	K	Joback Method
tc	692.33	K	Joback Method
tf	296.03	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.92	J/mol×K	534.18	Joback Method
cpg	550.22	J/mol×K	560.54	Joback Method
cpg	566.83	J/mol×K	586.90	Joback Method
cpg	582.76	J/mol×K	613.26	Joback Method
cpg	598.02	J/mol×K	639.62	Joback Method
cpg	612.62	J/mol×K	665.97	Joback Method
cpg	626.58	J/mol×K	692.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415441&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