Methylsulphonamide, N-ethyl-N-3-methylbutyl-

Inchi: InChI=1S/C8H19NO2S/c1-5-9(12(4,10)11)7-6-8(2)3/h8H,5-7H2,1-4H3
InchiKey: ZTOKWWWIRNEJPA-UHFFFAOYSA-N
Formula: C8H19NO2S
SMILES: CCN(CCC(C)C)S(C)(=O)=O
Mol. weight [g/mol]: 193.31

Physical Properties

Property code	Value	Unit	Source
gf	-343.72	kJ/mol	Joback Method
hf	-599.55	kJ/mol	Joback Method
hfus	27.35	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.314		Crippen Method
mcvol	161.650	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	442.22	K	Joback Method
tc	606.26	K	Joback Method
tf	235.95	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.26	J/mol×K	442.22	Joback Method
cpg	356.09	J/mol×K	469.56	Joback Method
cpg	370.35	J/mol×K	496.90	Joback Method
cpg	384.05	J/mol×K	524.24	Joback Method
cpg	397.19	J/mol×K	551.58	Joback Method
cpg	409.79	J/mol×K	578.92	Joback Method
cpg	421.84	J/mol×K	606.26	Joback Method

Sources

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=U415435&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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