Methylsulphonamide, N-ethyl-N-isobutyl-

Inchi: InChI=1S/C7H17NO2S/c1-5-8(6-7(2)3)11(4,9)10/h7H,5-6H2,1-4H3
InchiKey: VKAUPUOOPOJGEW-UHFFFAOYSA-N
Formula: C7H17NO2S
SMILES: CCN(CC(C)C)S(C)(=O)=O
Mol. weight [g/mol]: 179.28

Physical Properties

Property code	Value	Unit	Source
gf	-352.14	kJ/mol	Joback Method
hf	-578.91	kJ/mol	Joback Method
hfus	24.76	kJ/mol	Joback Method
hvap	51.47	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.924		Crippen Method
mcvol	147.560	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	419.34	K	Joback Method
tc	584.12	K	Joback Method
tf	224.68	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.17	J/mol×K	419.34	Joback Method
cpg	312.05	J/mol×K	446.80	Joback Method
cpg	325.41	J/mol×K	474.27	Joback Method
cpg	338.25	J/mol×K	501.73	Joback Method
cpg	350.58	J/mol×K	529.20	Joback Method
cpg	362.40	J/mol×K	556.66	Joback Method
cpg	373.73	J/mol×K	584.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415433&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

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