Methylsulphonamide, N-ethyl-N-butyl-

Inchi: InChI=1S/C7H17NO2S/c1-4-6-7-8(5-2)11(3,9)10/h4-7H2,1-3H3
InchiKey: WRRITKOTEHDDMZ-UHFFFAOYSA-N
Formula: C7H17NO2S
SMILES: CCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 179.28

Physical Properties

Property code	Value	Unit	Source
gf	-349.70	kJ/mol	Joback Method
hf	-573.63	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	51.85	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	1.068		Crippen Method
mcvol	147.560	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	419.78	K	Joback Method
tc	581.06	K	Joback Method
tf	239.68	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.19	J/mol×K	419.78	Joback Method
cpg	311.70	J/mol×K	446.66	Joback Method
cpg	324.71	J/mol×K	473.54	Joback Method
cpg	337.23	J/mol×K	500.42	Joback Method
cpg	349.27	J/mol×K	527.30	Joback Method
cpg	360.83	J/mol×K	554.18	Joback Method
cpg	371.91	J/mol×K	581.06	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=U415434&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

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