Methylsulphonamide, N-ethyl-N-heptyl-

Inchi: InChI=1S/C10H23NO2S/c1-4-6-7-8-9-10-11(5-2)14(3,12)13/h4-10H2,1-3H3
InchiKey: SPVNJZUGCVYGNQ-UHFFFAOYSA-N
Formula: C10H23NO2S
SMILES: CCCCCCCN(CC)S(C)(=O)=O
Mol. weight [g/mol]: 221.36

Physical Properties

Property code	Value	Unit	Source
gf	-324.44	kJ/mol	Joback Method
hf	-635.55	kJ/mol	Joback Method
hfus	36.05	kJ/mol	Joback Method
hvap	58.53	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.238		Crippen Method
mcvol	189.830	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
tb	488.42	K	Joback Method
tc	647.72	K	Joback Method
tf	273.49	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.40	J/mol×K	488.42	Joback Method
cpg	449.44	J/mol×K	514.97	Joback Method
cpg	464.86	J/mol×K	541.52	Joback Method
cpg	479.67	J/mol×K	568.07	Joback Method
cpg	493.87	J/mol×K	594.62	Joback Method
cpg	507.48	J/mol×K	621.17	Joback Method
cpg	520.51	J/mol×K	647.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415439&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