Pentamethylbenzenesulphonamide

Inchi: InChI=1S/C11H17NO2S/c1-6-7(2)9(4)11(15(12,13)14)10(5)8(6)3/h1-5H3,(H2,12,13,14)
InchiKey: QITSJCOOORWWSM-UHFFFAOYSA-N
Formula: C11H17NO2S
SMILES: Cc1c(C)c(C)c(S(N)(=O)=O)c(C)c1C
Mol. weight [g/mol]: 227.32
CAS: 208173-25-5

Physical Properties

Property code	Value	Unit	Source
gf	-296.09	kJ/mol	Joback Method
hf	-510.75	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	74.94	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	1.876		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	622.97	K	Joback Method
tc	832.32	K	Joback Method
tf	424.57	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.63	J/mol×K	622.97	Joback Method
cpg	458.97	J/mol×K	657.86	Joback Method
cpg	472.56	J/mol×K	692.75	Joback Method
cpg	485.38	J/mol×K	727.64	Joback Method
cpg	497.43	J/mol×K	762.54	Joback Method
cpg	508.70	J/mol×K	797.43	Joback Method
cpg	519.18	J/mol×K	832.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C208173255&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume