Ethylsulfonylpropanone

Inchi: InChI=1S/C5H10O3S/c1-3-9(7,8)4-5(2)6/h3-4H2,1-2H3
InchiKey: QZKCAVXRXZLZSJ-UHFFFAOYSA-N
Formula: C5H10O3S
SMILES: CCS(=O)(=O)CC(C)=O
Mol. weight [g/mol]: 150.20
CAS: 86453-13-6

Physical Properties

Property code	Value	Unit	Source
gf	-606.24	kJ/mol	Joback Method
hf	-712.46	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	52.11	kJ/mol	Joback Method
log10ws	-0.03		Crippen Method
logp	0.010		Crippen Method
mcvol	110.970	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
tb	415.45	K	Joback Method
tc	591.34	K	Joback Method
tf	234.60	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.19	J/mol×K	415.45	Joback Method
cpg	219.87	J/mol×K	444.76	Joback Method
cpg	229.21	J/mol×K	474.08	Joback Method
cpg	238.21	J/mol×K	503.39	Joback Method
cpg	246.87	J/mol×K	532.71	Joback Method
cpg	255.18	J/mol×K	562.02	Joback Method
cpg	263.14	J/mol×K	591.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86453136&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume