ISOPROPYL METHYL SULFONE

Other names: Isopropyl methyl sulphone
Inchi: InChI=1S/C4H10O2S/c1-4(2)7(3,5)6/h4H,1-3H3
InchiKey: VTWYQAQIXXAXOR-UHFFFAOYSA-N
Formula: C4H10O2S
SMILES: CC(C)S(C)(=O)=O
Mol. weight [g/mol]: 122.19

Physical Properties

Property code	Value	Unit	Source
chl	-3101.30 ± 0.63	kJ/mol	NIST Webbook
hf	-433.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-503.80 ± 1.30	kJ/mol	NIST Webbook
hfus	13.97	kJ/mol	Joback Method
hvap	70.00 ± 3.00	kJ/mol	NIST Webbook
ie	10.08	eV	Cheméo Relay (1.0)
logp	0.439		Crippen Method
mcvol	95.310	ml/mol	McGowan Method
tb	512.13	K	Cheméo Relay (1.0)
tf	289.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.92	J/mol×K	338.26	Joback Method
cpg	166.83	J/mol×K	366.04	Joback Method
cpg	175.49	J/mol×K	393.82	Joback Method
cpg	183.89	J/mol×K	421.61	Joback Method
cpg	192.04	J/mol×K	449.39	Joback Method
cpg	199.93	J/mol×K	477.17	Joback Method
cpg	207.56	J/mol×K	504.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4853741&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point