Methylsulfenyliodide

Inchi: InChI=1S/CH3IS/c1-3-2/h1H3
InchiKey: KMLSFWQTQIKPFQ-UHFFFAOYSA-N
Formula: CH3IS
SMILES: CSI
Mol. weight [g/mol]: 174.00
CAS: 86381-89-7

Physical Properties

Property code	Value	Unit	Source
gf	48.78	kJ/mol	Joback Method
hf	30.00 ± 3.10	kJ/mol	NIST Webbook
hfus	6.88	kJ/mol	Joback Method
hvap	34.01	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.699		Crippen Method
mcvol	67.120	ml/mol	McGowan Method
pc	5747.92	kPa	Joback Method
tb	384.20	K	Joback Method
tc	625.15	K	Joback Method
tf	193.49	K	Joback Method
vc	0.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.20	J/mol×K	384.20	Joback Method
cpg	77.44	J/mol×K	424.36	Joback Method
cpg	80.49	J/mol×K	464.52	Joback Method
cpg	83.38	J/mol×K	504.67	Joback Method
cpg	86.09	J/mol×K	544.83	Joback Method
cpg	88.64	J/mol×K	584.99	Joback Method
cpg	91.04	J/mol×K	625.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86381897&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