

Methanesulfonamide, iodo-

Inchi:	InChI=1S/CH4INO2S/c2-1-6(3,4)5/h1H2,(H2,3,4,5)
InchiKey:	FDGDRDDFTVNCGU-UHFFFAOYSA-N
Formula:	CH4INO2S
SMILES:	NS(=O)(=O)Cl
Mol. weight [g/mol]:	221.02
CAS:	22354-13-8

Physical Properties

Property code	Value	Unit	Source
gf	-386.43	kJ/mol	Joback Method
hf	-406.66	kJ/mol	Joback Method
hfus	19.33	kJ/mol	Joback Method
hvap	56.47	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	-0.333		Crippen Method
mcvol	88.840	ml/mol	McGowan Method
pc	7915.30	kPa	Joback Method
tb	435.73	K	Joback Method
tc	657.07	K	Joback Method
tf	280.91	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.04	J/molxK	435.73	Joback Method
cpg	142.38	J/molxK	472.62	Joback Method
cpg	147.42	J/molxK	509.51	Joback Method
cpg	152.17	J/molxK	546.40	Joback Method
cpg	156.62	J/molxK	583.29	Joback Method
cpg	160.78	J/molxK	620.18	Joback Method
cpg	164.63	J/molxK	657.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22354138&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

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