

4-Iodothioanisole

Inchi:	InChI=1S/C7H7IS/c1-9-7-4-2-6(8)3-5-7/h2-5H,1H3
InchiKey:	VGQFOKHFPSTYJY-UHFFFAOYSA-N
Formula:	C7H7IS
SMILES:	CSc1ccc(I)cc1
Mol. weight [g/mol]:	250.10
CAS:	35371-03-0

Physical Properties

Property code	Value	Unit	Source
gf	202.08	kJ/mol	Joback Method
hf	155.99	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	50.30	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.013		Crippen Method
mcvol	127.900	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	553.14	K	Joback Method
tc	830.50	K	Joback Method
tf	300.05	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.59	J/mol×K	553.14	Joback Method
cpg	234.27	J/mol×K	599.37	Joback Method
cpg	244.05	J/mol×K	645.59	Joback Method
cpg	252.98	J/mol×K	691.82	Joback Method
cpg	261.12	J/mol×K	738.05	Joback Method
cpg	268.51	J/mol×K	784.28	Joback Method
cpg	275.21	J/mol×K	830.50	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35371030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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