

2-Isopropylphenyl isothiocyanate

Inchi: InChI=1S/C10H11NS/c1-8(2)9-5-3-4-6-10(9)11-7-12/h3-6,8H,1-2H3
InchiKey: QQOQMDSEMQHMR-UHFFFAOYSA-N
Formula: C10H11NS
SMILES: CC(C)c1ccccc1N=C=S
Mol. weight [g/mol]: 177.27
CAS: 36176-31-5

Physical Properties

Property code	Value	Unit	Source
hf	254.12	kJ/mol	Joback Method
hvap	50.84	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.544		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	605.37	K	Joback Method
tc	860.42	K	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=C36176315&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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

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