

o-tolylthiourea

Inchi:	InChI=1S/C8H10N2S/c1-6-4-2-3-5-7(6)10-8(9)11/h2-5H,1H3,(H3,9,10,11)
InchiKey:	ACLZYRNSDLQOIA-UHFFFAOYSA-N
Formula:	C8H10N2S
SMILES:	Cc1ccccc1NC(N)=S
Mol. weight [g/mol]:	166.24
CAS:	614-78-8

Physical Properties

Property code	Value	Unit	Source
gf	392.16	kJ/mol	Joback Method
hf	250.37	kJ/mol	Joback Method
hfus	25.03	kJ/mol	Joback Method
hvap	60.15	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
log10ws	-2.74		Crippen Method
logp	1.651		Crippen Method
mcvol	131.830	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	606.84	K	Joback Method
tc	856.91	K	Joback Method
tf	389.05	K	Joback Method
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.68	J/mol×K	606.84	Joback Method
cpg	310.93	J/mol×K	648.52	Joback Method
cpg	321.26	J/mol×K	690.20	Joback Method
cpg	330.76	J/mol×K	731.88	Joback Method
cpg	339.53	J/mol×K	773.56	Joback Method
cpg	347.64	J/mol×K	815.23	Joback Method
cpg	355.21	J/mol×K	856.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C614788&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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