

Thiourea, (2-chlorophenyl)-

Other names:	Urea, 1-(o-chlorophenyl)-2-thio-(o-Chlorophenyl)thiourea N-(2-Chlorophenyl)thiourea 1-(o-Chlorophenyl)thiourea 1-(2-Chlorophenyl)-2-thiourea 1-(2-Chlorophenyl)thiourea 2-Chlorophenylthiourea Rcra waste number P026 NSC 1165 Thiourea, N-(2-chlorophenyl)-
Inchi:	InChI=1S/C7H7ClN2S/c8-5-3-1-2-4-6(5)10-7(9)11/h1-4H,(H3,9,10,11)
InchiKey:	YZUKKTCDYSIWKJ-UHFFFAOYSA-N
Formula:	C7H7ClN2S
SMILES:	NC(=S)Nc1ccccc1Cl
Mol. weight [g/mol]:	186.66
CAS:	5344-82-1

Physical Properties

Property code	Value	Unit	Source
gf	371.81	kJ/mol	Joback Method
hf	255.27	kJ/mol	Joback Method
hfus	26.63	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Joback Method
ie	8.05	eV	NIST Webbook
log10ws	-2.95		Crippen Method
logp	1.995		Crippen Method
mcvol	129.980	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	621.39	K	Joback Method
tc	880.43	K	Joback Method
tf	416.44 ± 0.20	K	NIST Webbook
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.33	J/mol×K	794.08	Joback Method
cpg	313.77	J/mol×K	837.25	Joback Method
cpg	275.13	J/mol×K	621.39	Joback Method
cpg	284.35	J/mol×K	664.56	Joback Method
cpg	292.72	J/mol×K	707.74	Joback Method
cpg	300.35	J/mol×K	750.91	Joback Method
cpg	319.77	J/mol×K	880.43	Joback Method
hfust	22.29	kJ/mol	413.50	NIST Webbook
hfust	22.29	kJ/mol	413.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5344821&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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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