2-(2-Chlorophenoxy)thioacetamide

Inchi: InChI=1S/C8H8ClNOS/c9-6-3-1-2-4-7(6)11-5-8(10)12/h1-4H,5H2,(H2,10,12)
InchiKey: YVAJKXSZBMTZMX-UHFFFAOYSA-N
Formula: C8H8ClNOS
SMILES: NC(=S)COc1ccccc1Cl
Mol. weight [g/mol]: 201.67
CAS: 35370-94-6

Physical Properties

Property code	Value	Unit	Source
gf	185.84	kJ/mol	Joback Method
hf	48.94	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.005		Crippen Method
mcvol	139.960	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	616.52	K	Joback Method
tc	868.49	K	Joback Method
tf	388.54	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.94	J/mol×K	616.52	Joback Method
cpg	310.05	J/mol×K	658.51	Joback Method
cpg	319.34	J/mol×K	700.51	Joback Method
cpg	327.89	J/mol×K	742.50	Joback Method
cpg	335.76	J/mol×K	784.50	Joback Method
cpg	343.03	J/mol×K	826.49	Joback Method
cpg	349.76	J/mol×K	868.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35370946&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