2,4-Dichlorophenyl-diethylthionocarbamate

Inchi: InChI=1S/C11H13Cl2NOS/c1-3-14(4-2)11(16)15-10-6-5-8(12)7-9(10)13/h5-7H,3-4H2,1-2
InchiKey: FWXFIMVQNOYOTD-UHFFFAOYSA-N
Formula: C11H13Cl2NOS
SMILES: CCN(CC)C(=S)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 278.20
CAS: 116401-19-5

Physical Properties

Property code	Value	Unit	Source
gf	233.87	kJ/mol	Joback Method
hf	-6.45	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	63.63	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.999		Crippen Method
mcvol	194.470	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	667.48	K	Joback Method
tc	897.72	K	Joback Method
tf	414.00	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.82	J/mol×K	667.48	Joback Method
cpg	459.21	J/mol×K	705.85	Joback Method
cpg	470.72	J/mol×K	744.23	Joback Method
cpg	481.43	J/mol×K	782.60	Joback Method
cpg	491.40	J/mol×K	820.97	Joback Method
cpg	500.70	J/mol×K	859.35	Joback Method
cpg	509.40	J/mol×K	897.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401195&Units=SI

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