N,N-Diethyl-S-(4-chlorophenyl) thiocarbamide

Inchi: InChI=1S/C11H15ClN2S/c1-3-14(4-2)11(13)15-10-7-5-9(12)6-8-10/h5-8,13H,3-4H2,1-2H
InchiKey: BTXGWQRGCOIDJR-UHFFFAOYSA-N
Formula: C11H15ClN2S
SMILES: CCN(CC)C(=N)Sc1ccc(Cl)cc1
Mol. weight [g/mol]: 242.77

Physical Properties

Property code	Value	Unit	Source
gf	480.09	kJ/mol	Joback Method
hf	246.68	kJ/mol	Joback Method
hvap	68.34	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.709		Crippen Method
mcvol	186.340	ml/mol	McGowan Method
rinpol	1979.00		NIST Webbook
tb	685.73	K	Joback Method
tf	418.24	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.70	J/mol×K	685.73	Joback Method
cpg	80.78	J/mol×K	100.12	Joback Method
cpg	80.78	J/mol×K	100.12	Joback Method
cpg	80.78	J/mol×K	100.12	Joback Method
cpg	80.78	J/mol×K	100.12	Joback Method
cpg	80.78	J/mol×K	100.12	Joback Method
cpg	80.78	J/mol×K	100.12	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=R537583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point