Acetamide, N-(3-chlorophenyl)-2-phenylthio-

Inchi: InChI=1S/C14H12ClNOS/c15-11-5-4-6-12(9-11)16-14(17)10-18-13-7-2-1-3-8-13/h1-9H,1
InchiKey: OTOSJZUVCFFPHN-UHFFFAOYSA-N
Formula: C14H12ClNOS
SMILES: O=C(CSc1ccccc1)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 277.77

Physical Properties

Property code	Value	Unit	Source
gf	263.85	kJ/mol	Joback Method
hf	96.32	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	76.36	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.071		Crippen Method
mcvol	200.740	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	788.31	K	Joback Method
tc	1050.02	K	Joback Method
tf	479.81	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.00	J/mol×K	788.31	Joback Method
cpg	525.45	J/mol×K	831.93	Joback Method
cpg	536.63	J/mol×K	875.55	Joback Method
cpg	546.62	J/mol×K	919.16	Joback Method
cpg	555.51	J/mol×K	962.78	Joback Method
cpg	563.37	J/mol×K	1006.40	Joback Method
cpg	570.30	J/mol×K	1050.02	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=U307207&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume