Propanamide, N-(3-chlorophenyl)-3-chloro-

Inchi: InChI=1S/C9H9Cl2NO/c10-5-4-9(13)12-8-3-1-2-7(11)6-8/h1-3,6H,4-5H2,(H,12,13)
InchiKey: PPDCJGYLZPSGAW-UHFFFAOYSA-N
Formula: C9H9Cl2NO
SMILES: O=C(CCCl)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 218.08

Physical Properties

Property code	Value	Unit	Source
gf	64.29	kJ/mol	Joback Method
hf	-94.62	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.907		Crippen Method
mcvol	149.940	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1861.00		NIST Webbook
tb	615.88	K	Joback Method
tc	843.79	K	Joback Method
tf	392.56	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.96	J/mol×K	615.88	Joback Method
cpg	336.85	J/mol×K	653.86	Joback Method
cpg	346.95	J/mol×K	691.85	Joback Method
cpg	356.31	J/mol×K	729.83	Joback Method
cpg	364.95	J/mol×K	767.82	Joback Method
cpg	372.92	J/mol×K	805.80	Joback Method
cpg	380.25	J/mol×K	843.79	Joback Method

Sources

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=U307227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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