Benzamide, 3-chloro-N-(3-chlorobenzoyl)-N-methyl-

Inchi: InChI=1S/C15H11Cl2NO2/c1-18(14(19)10-4-2-6-12(16)8-10)15(20)11-5-3-7-13(17)9-11/h
InchiKey: JBCJLTGZBXLDHD-UHFFFAOYSA-N
Formula: C15H11Cl2NO2
SMILES: CN(C(=O)c1cccc(Cl)c1)C(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 308.16

Physical Properties

Property code	Value	Unit	Source
gf	110.06	kJ/mol	Joback Method
hf	-91.92	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	79.17	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.906		Crippen Method
mcvol	212.290	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	800.96	K	Joback Method
tc	1049.58	K	Joback Method
tf	528.86	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.95	J/mol×K	800.96	Joback Method
cpg	548.38	J/mol×K	842.40	Joback Method
cpg	558.72	J/mol×K	883.83	Joback Method
cpg	568.06	J/mol×K	925.27	Joback Method
cpg	576.50	J/mol×K	966.71	Joback Method
cpg	584.11	J/mol×K	1008.15	Joback Method
cpg	590.98	J/mol×K	1049.58	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=U407988&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