Benzamide, 2-chloro-N-(2-chlorobenzoyl)-N-(3-methylbutyl)-

Inchi: InChI=1S/C19H19Cl2NO2/c1-13(2)11-12-22(18(23)14-7-3-5-9-16(14)20)19(24)15-8-4-6-

InchiKey: MRCRKXDVEBGBQY-UHFFFAOYSA-N

Formula: C19H19Cl2NO2

SMILES: CC(C)CCN(C(=O)c1ccccc1Cl)C(=O)c1ccccc1Cl

Mol. weight [g/mol]: 364.27

Physical Properties

Property code	Value	Unit	Source
gf	141.30	kJ/mol	Joback Method
hf	-179.76	kJ/mol	Joback Method
hfus	43.36	kJ/mol	Joback Method
hvap	87.68	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.322		Crippen Method
mcvol	268.650	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2556.00		NIST Webbook
rinpol	2556.00		NIST Webbook
tb	892.04	K	Joback Method
tc	1129.01	K	Joback Method
tf	558.94	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.32	J/mol×K	892.04	Joback Method
cpg	770.05	J/mol×K	931.54	Joback Method
cpg	781.68	J/mol×K	971.03	Joback Method
cpg	792.31	J/mol×K	1010.53	Joback Method
cpg	802.04	J/mol×K	1050.02	Joback Method
cpg	810.95	J/mol×K	1089.52	Joback Method
cpg	819.15	J/mol×K	1129.01	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=U407497&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