Benzamide, 2-chloro-N-(2-chlorobenzoyl)-N-isobutyl-

Inchi: InChI=1S/C18H17Cl2NO2/c1-12(2)11-21(17(22)13-7-3-5-9-15(13)19)18(23)14-8-4-6-10-

InchiKey: APTIVEZVNOVVQF-UHFFFAOYSA-N

Formula: C18H17Cl2NO2

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

Mol. weight [g/mol]: 350.24

Physical Properties

Property code	Value	Unit	Source
gf	132.88	kJ/mol	Joback Method
hf	-159.12	kJ/mol	Joback Method
hfus	40.77	kJ/mol	Joback Method
hvap	85.45	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	4.932		Crippen Method
mcvol	254.560	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	869.16	K	Joback Method
tc	1109.23	K	Joback Method
tf	547.67	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.03	J/mol×K	869.16	Joback Method
cpg	713.54	J/mol×K	909.17	Joback Method
cpg	724.95	J/mol×K	949.18	Joback Method
cpg	735.34	J/mol×K	989.19	Joback Method
cpg	744.81	J/mol×K	1029.20	Joback Method
cpg	753.45	J/mol×K	1069.22	Joback Method
cpg	761.35	J/mol×K	1109.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407495&Units=SI
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

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

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