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

Inchi: InChI=1S/C20H21Cl2NO2/c1-2-3-4-9-14-23(19(24)15-10-5-7-12-17(15)21)20(25)16-11-6

InchiKey: JPXOOXQKDRXSAU-UHFFFAOYSA-N

Formula: C20H21Cl2NO2

SMILES: CCCCCCN(C(=O)c1ccccc1Cl)C(=O)c1ccccc1Cl

Mol. weight [g/mol]: 378.29

Physical Properties

Property code	Value	Unit	Source
gf	152.16	kJ/mol	Joback Method
hf	-195.12	kJ/mol	Joback Method
hfus	49.47	kJ/mol	Joback Method
hvap	90.30	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.856		Crippen Method
mcvol	282.740	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2713.00		NIST Webbook
rinpol	2713.00		NIST Webbook
tb	915.36	K	Joback Method
tc	1147.09	K	Joback Method
tf	585.21	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.90	J/mol×K	915.36	Joback Method
cpg	826.71	J/mol×K	953.98	Joback Method
cpg	838.48	J/mol×K	992.60	Joback Method
cpg	849.30	J/mol×K	1031.23	Joback Method
cpg	859.27	J/mol×K	1069.85	Joback Method
cpg	868.46	J/mol×K	1108.47	Joback Method
cpg	876.99	J/mol×K	1147.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407499&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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