

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

Inchi:	InChI=1S/C23H27Cl2NO2/c1-2-3-4-5-6-7-12-17-26(22(27)18-13-8-10-15-20(18)24)23(28)
InchiKey:	PUFRFPNSRVTTTRW-UHFFFAOYSA-N
Formula:	C23H27Cl2NO2
SMILES:	CCCCCCCCCN(C(=O)c1ccccc1Cl)C(=O)c1ccccc1Cl
Mol. weight [g/mol]:	420.37

Physical Properties

Property code	Value	Unit	Source
gf	177.42	kJ/mol	Joback Method
hf	-257.04	kJ/mol	Joback Method
hfus	57.24	kJ/mol	Joback Method
hvap	96.97	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.027		Crippen Method
mcvol	325.010	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	3036.00		NIST Webbook
rinpol	3036.00		NIST Webbook
tb	984.00	K	Joback Method
tc	1214.33	K	Joback Method
tf	619.02	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.65	J/molxK	984.00	Joback Method
cpg	1003.12	J/molxK	1022.39	Joback Method
cpg	1015.57	J/molxK	1060.78	Joback Method
cpg	1027.08	J/molxK	1099.16	Joback Method
cpg	1037.78	J/molxK	1137.55	Joback Method
cpg	1047.76	J/molxK	1175.94	Joback Method
cpg	1057.11	J/molxK	1214.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U407503&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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