

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

Inchi:	InChI=1S/C19H19Cl2NO2/c1-2-3-8-13-22(18(23)14-9-4-6-11-16(14)20)19(24)15-10-5-7-
InchiKey:	PTHFHLVQJKXVNI-UHFFFAOYSA-N
Formula:	C19H19Cl2NO2
SMILES:	CCCCCN(C(=O)c1ccccc1Cl)C(=O)c1ccccc1Cl
Mol. weight [g/mol]:	364.27

Physical Properties

Property code	Value	Unit	Source
gf	143.74	kJ/mol	Joback Method
hf	-174.48	kJ/mol	Joback Method
hfus	46.88	kJ/mol	Joback Method
hvap	88.07	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.466		Crippen Method
mcvol	268.650	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpola	2609.00		NIST Webbook
rinpola	2609.00		NIST Webbook
tb	892.48	K	Joback Method
tc	1126.24	K	Joback Method
tf	573.94	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.77	J/molxK	892.48	Joback Method
cpg	769.37	J/molxK	931.44	Joback Method
cpg	780.91	J/molxK	970.40	Joback Method
cpg	791.49	J/molxK	1009.36	Joback Method
cpg	801.21	J/molxK	1048.32	Joback Method
cpg	810.14	J/molxK	1087.28	Joback Method
cpg	818.38	J/molxK	1126.24	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=U407498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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