

2-Chloro-1,4-dibenzamido benzene

Other names:	Benzene, 1,4-bis(benzoylamino)-2-chloro-
Inchi:	InChI=1S/C20H15ClN2O2/c21-17-13-16(22-19(24)14-7-3-1-4-8-14)11-12-18(17)23-20(2)
InchiKey:	AUCDGWBCUYSRAV-UHFFFAOYSA-N
Formula:	C20H15ClN2O2
SMILES:	O=C(Nc1ccc(NC(=O)c2ccccc2)c(Cl)c1)c1ccccc1
Mol. weight [g/mol]:	350.80
CAS:	300360-38-7

Physical Properties

Property code	Value	Unit	Source
gf	344.50	kJ/mol	Joback Method
hf	96.56	kJ/mol	Joback Method
hfus	46.49	kJ/mol	Joback Method
hvap	99.02	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.845		Crippen Method
mcvol	256.720	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	992.51	K	Joback Method
tc	1253.87	K	Joback Method
tf	654.56	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.77	J/mol×K	992.51	Joback Method
cpg	757.84	J/mol×K	1036.07	Joback Method
cpg	766.85	J/mol×K	1079.63	Joback Method
cpg	774.94	J/mol×K	1123.19	Joback Method
cpg	782.23	J/mol×K	1166.75	Joback Method
cpg	788.86	J/mol×K	1210.31	Joback Method
cpg	794.95	J/mol×K	1253.87	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=C300360387&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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