

Benzene, 1,4-bis(benzoylamino)-2-chloro-

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

Physical Properties

Property code	Value	Unit	Source
hf	-52.93	kJ/mol	Cheméo Relay (1.0)
hfus	46.49	kJ/mol	Joback Method
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-5.60		Cheméo Relay (1.0)
logp	4.845		Crippen Method
mcvol	256.720	ml/mol	McGowan Method
tf	464.01	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C300360387&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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