

N-(4-bromo-phenyl)-2-chloro-benzamide

Other names:	Benzamide, N-(4-bromophenyl)-2-chloro-
Inchi:	InChI=1S/C13H9BrClNO/c14-9-5-7-10(8-6-9)16-13(17)11-3-1-2-4-12(11)15/h1-8H,(H,16,
InchiKey:	KQUDDDBZEDXTSPT-UHFFFAOYSA-N
Formula:	C13H9BrClNO
SMILES:	O=C(Nc1ccc(Br)cc1)c1ccccc1Cl
Mol. weight [g/mol]:	310.58

Physical Properties

Property code	Value	Unit	Source
hf	8.18	kJ/mol	Cheméo Relay (1.0)
hfus	32.91	kJ/mol	Joback Method
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-5.11		Cheméo Relay (1.0)
logp	4.355		Crippen Method
mcvol	187.800	ml/mol	McGowan Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	641.72	K	Cheméo Relay (1.0)
tf	436.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.57	J/mol×K	767.79	Joback Method
cpg	453.58	J/mol×K	811.64	Joback Method
cpg	463.54	J/mol×K	855.50	Joback Method
cpg	472.54	J/mol×K	899.35	Joback Method
cpg	480.69	J/mol×K	943.20	Joback Method
cpg	488.08	J/mol×K	987.06	Joback Method
cpg	494.80	J/mol×K	1030.91	Joback Method

Sources

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66569059&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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