

4-Chlorobenzamide, N-(4-chlorobenzoyl)-N-butyl-

Inchi:	InChI=1S/C18H17Cl2NO2/c1-2-3-12-21(17(22)13-4-8-15(19)9-5-13)18(23)14-6-10-16(20)
InchiKey:	AYTMNLJCFKOITC-UHFFFAOYSA-N
Formula:	C18H17Cl2NO2
SMILES:	CCCCN(C(=O)c1ccc(Cl)cc1)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	350.24

Physical Properties

Property code	Value	Unit	Source
gf	135.32	kJ/mol	Joback Method
hf	-153.84	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	85.84	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.076		Crippen Method
mvol	254.560	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	869.60	K	Joback Method
tc	1106.11	K	Joback Method
tf	562.67	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.46	J/molxK	869.60	Joback Method
cpg	712.82	J/molxK	909.02	Joback Method
cpg	724.12	J/molxK	948.44	Joback Method
cpg	734.44	J/molxK	987.85	Joback Method
cpg	743.89	J/molxK	1027.27	Joback Method
cpg	752.54	J/molxK	1066.69	Joback Method
cpg	760.49	J/molxK	1106.11	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=U407103&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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