4-Chloroacetamidobenzophenone

Other names:	Benzophenone, 2-acetamino-5-chloro-
	N-(2-Benzoyl-4-chlorophenyl)acetamide
	2-Amino-5-chlorobenzophenone, acetylated
	Diazepam, M(oxa/epam), acid hydrolyzed, acetylated
Inchi:	InChI=1S/C15H12ClNO2/c1-10(18)17-14-8-7-12(16)9-13(14)15(19)11-5-3-2-4-6-11/h2-9
InchiKey:	NHAUKYAYIYDFST-UHFFFAOYSA-N
Formula:	C15H12ClNO2
SMILES:	CC(=O)Nc1ccc(Cl)cc1C(=O)c1ccccc1
Mol. weight [g/mol]:	273.71
CAS:	13788-59-5

Physical Properties

Property code	Value	Unit	Source
gf	100.60	kJ/mol	Joback Method
hf	-90.24	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	79.17	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.529		Crippen Method
mcvol	200.050	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
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rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	801.26	K	Joback Method
tc	1048.65	K	Joback Method

tf	519.13	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.68	J/mol×K	801.26	Joback Method
cpg	537.52	J/mol×K	842.49	Joback Method
cpg	548.26	J/mol×K	883.72	Joback Method
cpg	557.97	J/mol×K	924.95	Joback Method
cpg	566.74	J/mol×K	966.18	Joback Method
cpg	574.62	J/mol×K	1007.41	Joback Method
cpg	581.68	J/mol×K	1048.65	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13788595&Units=SI
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

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume