Benzophenone, 2-acetamino-2',5-dichloro-

Other names: Cloxazolam M (delorazepam), hydrolysis, acetylated
Inchi: InChI=1S/C15H11Cl2NO2/c1-9(19)18-14-7-6-10(16)8-12(14)15(20)11-4-2-3-5-13(11)17/
InchiKey: UFFQVZHDIPJFDP-UHFFFAOYSA-N
Formula: C15H11Cl2NO2
SMILES: CC(=O)Nc1ccc(Cl)cc1C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 308.16
CAS: 289504-18-3

Physical Properties

Property code	Value	Unit	Source
gf	79.04	kJ/mol	Joback Method
hf	-117.45	kJ/mol	Joback Method
hfus	38.21	kJ/mol	Joback Method
hvap	84.22	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.183		Crippen Method
mcvol	212.290	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	843.67	K	Joback Method
tc	1093.63	K	Joback Method
tf	561.57	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.22	J/mol×K	843.67	Joback Method
cpg	554.71	J/mol×K	885.33	Joback Method
cpg	564.18	J/mol×K	926.99	Joback Method
cpg	572.68	J/mol×K	968.65	Joback Method

cpg	580.29	J/mol×K	1010.31	Joback Method
cpg	587.08	J/mol×K	1051.97	Joback Method
cpg	593.09	J/mol×K	1093.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C289504183&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

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