Methanone, [5-chloro-2-(methylamino)phenyl](2-chlorophenyl)

Other names: Benzophenone, 2',5-dichloro-2-methylamino-
2-Methylamino-2',5-dichlorobenzophenone
2-methylamino-2',5-dichlor-benzophenone
2-Methylamino-5,2'-dichlorobenzophenone
2',5-dichloro-2-(methylamino)benzophenone

Inchi: InChI=1S/C14H11Cl2NO/c1-17-13-7-6-9(15)8-11(13)14(18)10-4-2-3-5-12(10)16/h2-8,17H

InchiKey: DQYHYPVCQHTLRO-UHFFFAOYSA-N

Formula: C14H11Cl2NO

SMILES: CNc1ccc(Cl)cc1C(=O)c1ccccc1Cl

Mol. weight [g/mol]: 280.15

CAS: 5621-86-3

Physical Properties

Property code	Value	Unit	Source
gf	199.54	kJ/mol	Joback Method
hf	15.77	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	75.25	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.266		Crippen Method
mcvol	196.630	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	766.92	K	Joback Method
tc	1017.40	K	Joback Method
tf	500.37	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.84	J/mol×K	766.92	Joback Method
cpg	495.76	J/mol×K	808.67	Joback Method
cpg	506.62	J/mol×K	850.41	Joback Method
cpg	516.49	J/mol×K	892.16	Joback Method
cpg	525.44	J/mol×K	933.91	Joback Method
cpg	533.53	J/mol×K	975.65	Joback Method
cpg	540.83	J/mol×K	1017.40	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5621863&Units=SI

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