Methanone, [5-chloro-2-[(cyclopropylmethyl)amino]phenyl]ph

Other names: 2-(Cyclopropyl-methyl)amino-5-chlor-benzophenone
2-[(Cyclopropylmethyl)amino]-5-chlorobenzophenone
Benzophenone, 2-cyclopropylmethylamino-5-chloro
Benzophenone, 5-chloro-2-cyclopropylmethylamino

Inchi: InChI=1S/C17H16ClNO/c18-14-8-9-16(19-11-12-6-7-12)15(10-14)17(20)13-4-2-1-3-5-13

InchiKey: WCRKZICZCPHVAB-UHFFFAOYSA-N

Formula: C17H16ClNO

SMILES: O=C(c1ccccc1)c1cc(Cl)ccc1NCC1CC1

Mol. weight [g/mol]: 285.77

CAS: 2897-00-9

Physical Properties

Property code	Value	Unit	Source
gf	307.11	kJ/mol	Joback Method
hf	53.86	kJ/mol	Joback Method
hfus	36.12	kJ/mol	Joback Method
hvap	76.79	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.393		Crippen Method
mcvol	215.800	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2398.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2385.00		NIST Webbook
rinpol	2407.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	799.89	K	Joback Method
tc	1047.48	K	Joback Method
tf	509.68	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.07	J/mol×K	799.89	Joback Method
cpg	620.65	J/mol×K	841.16	Joback Method
cpg	634.08	J/mol×K	882.42	Joback Method
cpg	646.48	J/mol×K	923.69	Joback Method
cpg	657.99	J/mol×K	964.95	Joback Method
cpg	668.74	J/mol×K	1006.22	Joback Method
cpg	678.84	J/mol×K	1047.48	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=C2897009&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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