5-Chloro-2'-fluoro-2-diethyaminoethylaminobenzo

Other names:	2-[2-(Diethylamino-ethylamino]-5-chloro-2'-fluorobenzophenone
	2-Diethylamino-ethylamino-5-chloro-2'-fluoro-benzophenone
	Benzophenone, 5-chloro-2-diethylaminoethylamino-2'-fluoro
	2-diethylamino-ethylamino-5-chlor-2'-fluor-benzophenone
Inchi:	InChI=1S/C19H22ClFN2O/c1-3-23(4-2)12-11-22-18-10-9-14(20)13-16(18)19(24)15-7-5-6
InchiKey:	VOXNSVGFHTWQLC-UHFFFAOYSA-N
Formula:	C19H22ClFN2O
SMILES:	CCN(CC)CCNc1ccc(Cl)cc1C(=O)c1ccccc1F
Mol. weight [g/mol]:	348.84
CAS:	36105-18-7

Physical Properties

Property code	Value	Unit	Source
gf	169.54	kJ/mol	Joback Method
hf	-200.27	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	83.22	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.464		Crippen Method
mcvol	266.590	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
rinpol	2555.00		NIST Webbook
rinpol	2555.00		NIST Webbook
rinpol	2558.00		NIST Webbook
rinpol	2555.00		NIST Webbook
rinpol	2555.00		NIST Webbook
rinpol	2560.00		NIST Webbook
tb	855.60	K	Joback Method
tc	1074.70	K	Joback Method
tf	559.86	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.52	J/mol×K	855.60	Joback Method
cpg	796.69	J/mol×K	892.12	Joback Method
cpg	809.81	J/mol×K	928.63	Joback Method
cpg	821.94	J/mol×K	965.15	Joback Method
cpg	833.16	J/mol×K	1001.67	Joback Method
cpg	843.54	J/mol×K	1038.18	Joback Method
cpg	853.15	J/mol×K	1074.70	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36105187&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.