5-Chloro-2'-fluoro-2-hydroxyethyaminobenzopher

Other names: 2-Hydroxyethylamino-5-chlor-2'-fluor-benzophenone
Inchi: InChI=1S/C15H13ClFNO2/c16-10-5-6-14(18-7-8-19)12(9-10)15(20)11-3-1-2-4-13(11)17/
InchiKey: CKDXNSUKTLFLRM-UHFFFAOYSA-N
Formula: C15H13ClFNO2
SMILES: O=C(c1ccccc1F)c1cc(Cl)ccc1NCCO
Mol. weight [g/mol]: 293.72
CAS: 35231-38-0

Physical Properties

Property code	Value	Unit	Source
gf	-111.74	kJ/mol	Joback Method
hf	-337.47	kJ/mol	Joback Method
hfus	39.58	kJ/mol	Joback Method
hvap	88.95	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.114		Crippen Method
mcvol	206.120	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	843.82	K	Joback Method
tc	1063.39	K	Joback Method
tf	543.13	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.07	J/mol×K	843.82	Joback Method
cpg	579.21	J/mol×K	880.41	Joback Method
cpg	588.54	J/mol×K	917.01	Joback Method
cpg	597.10	J/mol×K	953.60	Joback Method
cpg	604.95	J/mol×K	990.20	Joback Method
cpg	612.14	J/mol×K	1026.79	Joback Method

cpg	618.72	J/mol×K	1063.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35231380&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