Chlorflurecol methyl ester

Other names:	2-Chloro-9-hydroxy-9H-fluorene-9-carboxylic acid methyl ester
	9H-Fluorene-9-carboxylic acid, 2-chloro-9-hydroxy-, methyl ester
	CF 125
	CME 74050
	Chlorfluorenolmethyl
	Chlorflurecol-methyl
	Chlorflurenol methyl
	Chlorflurenol methyl ester
	Chloroflurenol methyl
	Chloroflurenol methyl ester
	EMD 7301
	EMD 7301W
	EMD-IT 3456
	Fluorene-9-carboxylic acid, 2-chloro-9-hydroxy-, methyl ester
	IT 3456
	Maintain
	Maintain A
	Maintain CF 125
	Methyl 2-chloro-9-hydroxyfluorene-9-carboxylate
	Methyl morphactin
	Morphactin
	Morphactin IT 3456
	Morphactine IT 3456
	TH 417-H
	chlorflurenol
Inchi:	InChI=1S/C15H11ClO3/c1-19-14(17)15(18)12-5-3-2-4-10(12)11-7-6-9(16)8-13(11)15/h2-
InchiKey:	LINPVWIEWJTEEJ-UHFFFAOYSA-N
Formula:	C15H11ClO3
SMILES:	COC(=O)C1(O)c2ccccc2-c2ccc(Cl)cc21
Mol. weight [g/mol]:	274.70
CAS:	2536-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-31.86	kJ/mol	Joback Method
hf	-226.69	kJ/mol	Joback Method

hfus	28.63	kJ/mol	Joback Method
hvap	84.16	kJ/mol	Joback Method
log10ws	-4.18		Aqueous Solubility Prediction Method
logp	2.729		Crippen Method
mcvol	189.380	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	815.24	K	Joback Method
tc	1047.29	K	Joback Method
tf	560.99	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.80	J/mol×K	815.24	Joback Method
cpg	520.21	J/mol×K	853.91	Joback Method
cpg	531.62	J/mol×K	892.59	Joback Method
cpg	543.24	J/mol×K	931.26	Joback Method
cpg	555.26	J/mol×K	969.94	Joback Method
cpg	567.86	J/mol×K	1008.61	Joback Method
cpg	581.24	J/mol×K	1047.29	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2536314&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume