

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 Chlorfluorenlmethyl Chlorflurecol-methyl Chlorflurenol methyl Chlorflurenol methyl ester Chlorofluorenol methyl Chlorofluorenol 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
mcpvol	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	m ³ /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

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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

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

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