Flurenol butyl ester

Other names:	9H-Fluorene-9-carboxylic acid, 9-hydroxy-, butyl ester
	Fluorene-9-carboxylic acid, 9-hydroxy-, butyl ester
	Butyl morphactin
	Butyl 9-hydroxy-9-fluorenecarboxylate
	Butyl 9-hydroxyfluorene-9-carboxylate
	Butyl 9-hydroxyfluorenyl-9-carboxylate
	Butyl ester of 9-hydroxyfluorene-9-carboxylic acid
	EMD 7311 W
	Flurecol-Butyl
	Flurenol ester
	IT 3233
	Morphactin IT 3233
	TH 407-H
	Flurenol-n-butyl ester
	9-Hydroxyfluorene-9-Carboxylic acid butyl ester
	9-Hydroxyfluorene-9-carboxylic acid n-butyl ester
	Flurenol-butyl
	Butyl flurenol
	butyl 9-hydroxy-9H-fluorene-9-carboxylate
Inchi:	InChI=1S/C18H18O3/c1-2-3-12-21-17(19)18(20)15-10-6-4-8-13(15)14-9-5-7-11-16(14)18
InchiKey:	PSGPXWYGJGGEEG-UHFFFAOYSA-N
Formula:	C18H18O3
SMILES:	CCCCOC(=O)C1(O)c2ccccc2-c2ccccc21
Mol. weight [g/mol]:	282.33
CAS:	2314-09-2

Physical Properties

Property code	Value	Unit	Source
gf	14.96	kJ/mol	Joback Method
hf	-261.40	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	85.79	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.246		Crippen Method
mcvol	219.410	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
tb	841.47	K	Joback Method

tc	1061.75	K	Joback Method
tf	344.68 ± 0.20	K	NIST Webbook
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.96	J/mol×K	841.47	Joback Method
cpg	667.12	J/mol×K	878.18	Joback Method
cpg	681.20	J/mol×K	914.90	Joback Method
cpg	695.38	J/mol×K	951.61	Joback Method
cpg	709.85	J/mol×K	988.32	Joback Method
cpg	724.77	J/mol×K	1025.04	Joback Method
cpg	740.33	J/mol×K	1061.75	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2314092&Units=SI

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