9H-Fluorene-9-carboxylic acid, 9-hydroxy-, butyl ester

Other names: 9-Hydroxyfluorene-9-Carboxylic acid butyl ester
9-Hydroxyfluorene-9-carboxylic acid n-butyl ester
9H-Fluorene-9-carboxylic acid, 9-hydroxy-, butyl ester
Butyl 9-hydroxy-9-fluorenecarboxylate
Butyl 9-hydroxyfluorene-9-carboxylate
Butyl 9-hydroxyfluorenyl-9-carboxylate
Butyl ester of 9-hydroxyfluorene-9-carboxylic acid
Butyl flurenol
Butyl morphactin
EMD 7311 W
Fluorene-9-carboxylic acid, 9-hydroxy-, butyl ester
Flurecol-Butyl
Flurenol ester
Flurenol-butyl
Flurenol-n-butyl ester
IT 3233
Morphactin IT 3233
TH 407-H
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]: 282.34

Physical Properties

Property code	Value	Unit	Source
af	0.8386		Cheméo Relay (1.0)
hf	-377.30	kJ/mol	Cheméo Relay (1.0)
hfus	32.59	kJ/mol	Joback Method
hvap	102.82	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.25		Cheméo Relay (1.0)
logp	3.246		Crippen Method
mcvol	219.410	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
tb	638.81	K	Cheméo Relay (1.0)
tc	941.75	K	Cheméo Relay (1.0)

tf	344.68 ± 0.20	K	NIST Webbook
vc	0.809	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2314092&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
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