2H-Naphtho[1,2-b]pyran-5-carboxylate, 2,2-dimethyl-6-hydroxy-

Other names: Mollugin
Inchi: InChI=1S/C17H16O4/c1-17(2)9-8-12-13(16(19)20-3)14(18)10-6-4-5-7-11(10)15(12)21-17
InchiKey: VLGATXOTCNBWIT-UHFFFAOYSA-N
Formula: C17H16O4
SMILES: COC(=O)c1c2c(c3ccccc3c1O)OC(C)(C)C=C2
Mol. weight [g/mol]: 284.31

Physical Properties

Property code	Value	Unit	Source
hfus	37.19	kJ/mol	Joback Method
logp	3.516		Crippen Method
mcvol	211.190	ml/mol	McGowan Method
rinpol	2237.00		NIST Webbook
rinpol	2237.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.94	J/mol×K	843.23	Joback Method
cpg	640.31	J/mol×K	884.81	Joback Method
cpg	655.91	J/mol×K	926.39	Joback Method
cpg	672.02	J/mol×K	967.97	Joback Method
cpg	688.91	J/mol×K	1009.54	Joback Method
cpg	706.88	J/mol×K	1051.12	Joback Method
cpg	726.20	J/mol×K	1092.70	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55481884&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices