2-Naphthalenecarboxylic acid, 3-hydroxy-, methyl ester

Other names: 2-Naphthoic acid, 3-hydroxy-, methyl ester
Methyl 3-hydroxy-2-naphthalenecarboxylate
Methyl 3-hydroxy-2-naphthoate
2-Hydroxy-3-naphthoic acid methyl ester
«beta»-Hydroxynaphthoic acid methyl ester

Inchi: InChI=1S/C12H10O3/c1-15-12(14)10-6-8-4-2-3-5-9(8)7-11(10)13/h2-7,13H,1H3

InchiKey: YVVBECLPRBAATK-UHFFFAOYSA-N

Formula: C12H10O3

SMILES: COC(=O)c1cc2ccccc2cc1O

Mol. weight [g/mol]: 202.21

CAS: 883-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-128.95	kJ/mol	Joback Method
hf	-296.99	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	69.05	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.332		Crippen Method
mcvol	150.030	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
tb	681.51	K	Joback Method
tc	925.21	K	Joback Method
tf	480.52	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.37	J/mol×K	681.51	Joback Method
cpg	393.77	J/mol×K	722.13	Joback Method
cpg	404.35	J/mol×K	762.74	Joback Method
cpg	414.25	J/mol×K	803.36	Joback Method

cpg	423.56	J/mol×K	843.97	Joback Method
cpg	432.41	J/mol×K	884.59	Joback Method
cpg	440.90	J/mol×K	925.21	Joback Method
dvisc	0.0003749	Pa×s	480.52	Joback Method
dvisc	0.0002178	Pa×s	514.02	Joback Method
dvisc	0.0001352	Pa×s	547.52	Joback Method
dvisc	0.0000886	Pa×s	581.01	Joback Method
dvisc	0.0000609	Pa×s	614.51	Joback Method
dvisc	0.0000435	Pa×s	648.01	Joback Method
dvisc	0.0000321	Pa×s	681.51	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=C883998&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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