1-Naphthol, isoBOC

Inchi: InChI=1S/C15H16O3/c1-11(2)10-17-15(16)18-14-9-5-7-12-6-3-4-8-13(12)14/h3-9,11H,10
InchiKey: UBAMHKZYHOHSLK-UHFFFAOYSA-N
Formula: C15H16O3
SMILES: CC(C)COC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 244.29

Physical Properties

Property code	Value	Unit	Source
gf	-56.51	kJ/mol	Joback Method
hf	-319.10	kJ/mol	Joback Method
hfus	25.73	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.011		Crippen Method
mcvol	192.300	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1895.00		NIST Webbook
tb	691.51	K	Joback Method
tc	915.00	K	Joback Method
tf	409.84	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.44	J/mol×K	691.51	Joback Method
cpg	526.47	J/mol×K	728.76	Joback Method
cpg	540.48	J/mol×K	766.01	Joback Method
cpg	553.49	J/mol×K	803.26	Joback Method
cpg	565.55	J/mol×K	840.50	Joback Method
cpg	576.70	J/mol×K	877.75	Joback Method
cpg	586.98	J/mol×K	915.00	Joback Method
dvisc	0.0011936	Pa×s	409.84	Joback Method
dvisc	0.0007346	Pa×s	456.79	Joback Method

dvisc	0.0004950	Pa×s	503.73	Joback Method
dvisc	0.0003567	Pa×s	550.67	Joback Method
dvisc	0.0002706	Pa×s	597.62	Joback Method
dvisc	0.0002138	Pa×s	644.57	Joback Method
dvisc	0.0001743	Pa×s	691.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R234878&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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