

2-Hydroxy-4-isopropynaphthalene

Inchi:	InChI=1S/C13H14O/c1-9(2)13-8-11(14)7-10-5-3-4-6-12(10)13/h3-9,14H,1-2H3
InchiKey:	SQWZYHJSSCQDRJ-UHFFFAOYSA-N
Formula:	C13H14O
SMILES:	CC(C)c1cc(O)cc2ccccc12
Mol. weight [g/mol]:	186.25
CAS:	162050-75-1

Physical Properties

Property code	Value	Unit	Source
gf	110.95	kJ/mol	Joback Method
hf	-78.11	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.669		Crippen Method
mvol	156.680	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1484.00		NIST Webbook
tb	627.66	K	Joback Method
tc	869.03	K	Joback Method
tf	404.63	K	Joback Method
vc	0.537	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.78	J/molxK	627.66	Joback Method
cpg	458.10	J/molxK	828.81	Joback Method
cpg	447.19	J/molxK	788.58	Joback Method
cpg	435.65	J/molxK	748.35	Joback Method
cpg	423.33	J/molxK	708.12	Joback Method
cpg	410.08	J/molxK	667.89	Joback Method
cpg	468.50	J/molxK	869.03	Joback Method

dvisc	0.0000412	Paxs	627.66	Joback Method
dvisc	0.0000601	Paxs	590.49	Joback Method
dvisc	0.0000923	Paxs	553.32	Joback Method
dvisc	0.0001507	Paxs	516.14	Joback Method
dvisc	0.0002656	Paxs	478.97	Joback Method
dvisc	0.0005150	Paxs	441.80	Joback Method
dvisc	0.0011279	Paxs	404.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C162050751&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

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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