

1-Naphthol, 5,7-dimethyl-

Other names:	5,7-Dimethyl-1-naphthol
Inchi:	InChI=1S/C12H12O/c1-8-6-9(2)10-4-3-5-12(13)11(10)7-8/h3-7,13H,1-2H3
InchiKey:	ZMYBSCDKKBZCTM-UHFFFAOYSA-N
Formula:	C12H12O
SMILES:	<chem>Cc1cc(C)c2cccc(O)c2c1</chem>
Mol. weight [g/mol]:	172.22
CAS:	31706-76-0

Physical Properties

Property code	Value	Unit	Source
gf	95.34	kJ/mol	Joback Method
hf	-63.66	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Joback Method
hvap	60.56	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.162		Crippen Method
mcvol	142.590	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
rinpol	1586.00		NIST Webbook
tb	610.20	K	Joback Method
tc	852.46	K	Joback Method
tf	420.88	K	Joback Method
vc	0.487	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.39	J/mol×K	610.20	Joback Method
cpg	359.36	J/mol×K	650.58	Joback Method
cpg	371.39	J/mol×K	690.95	Joback Method
cpg	382.59	J/mol×K	731.33	Joback Method
cpg	393.09	J/mol×K	771.71	Joback Method
cpg	403.02	J/mol×K	812.08	Joback Method
cpg	412.51	J/mol×K	852.46	Joback Method

dvisc	0.0007218	Paxs	420.88	Joback Method
dvisc	0.0003984	Paxs	452.43	Joback Method
dvisc	0.0002376	Paxs	483.99	Joback Method
dvisc	0.0001510	Paxs	515.54	Joback Method
dvisc	0.0001011	Paxs	547.09	Joback Method
dvisc	0.0000707	Paxs	578.65	Joback Method
dvisc	0.0000513	Paxs	610.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31706760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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