

NAPHTHALENE, 2,3-DIMETHOXY-

Other names:	2,3-Dimethoxynaphthalene
	2,3-Dihydroxynaphthalene, dimethyl ether
Inchi:	InChI=1S/C12H12O2/c1-13-11-7-9-5-3-4-6-10(9)8-12(11)14-2/h3-8H,1-2H3
InchiKey:	XYRPWXOJBNGTMX-UHFFFAOYSA-N
Formula:	C12H12O2
SMILES:	COc1cc2ccccc2cc1OC
Mol. weight [g/mol]:	188.23

Physical Properties

Property code	Value	Unit	Source
af	0.5473		Cheméo Relay (1.0)
gf	39.96	kJ/mol	Joback Method
hf	-126.77	kJ/mol	Cheméo Relay (1.0)
hfus	19.49	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Cheméo Relay (1.0)
ie	7.58	eV	Cheméo Relay (1.0)
log10ws	-3.88		Cheméo Relay (1.0)
logp	2.857		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1735.50		NIST Webbook
ripol	2239.00		NIST Webbook
tb	581.36	K	Cheméo Relay (1.0)
tc	813.67	K	Cheméo Relay (1.0)
tf	388.60	K	Cheméo Relay (1.0)
vc	0.549	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.34	J/mol×K	574.42	Joback Method
cpg	358.48	J/mol×K	612.02	Joback Method
cpg	371.78	J/mol×K	649.61	Joback Method
cpg	384.27	J/mol×K	687.21	Joback Method

cpg	395.97	J/mol×K	724.81	Joback Method
cpg	406.91	J/mol×K	762.41	Joback Method
cpg	417.11	J/mol×K	800.00	Joback Method
dvisc	0.0009014	Pa×s	353.62	Joback Method
dvisc	0.0006344	Pa×s	390.42	Joback Method
dvisc	0.0004743	Pa×s	427.22	Joback Method
dvisc	0.0003714	Pa×s	464.02	Joback Method
dvisc	0.0003014	Pa×s	500.82	Joback Method
dvisc	0.0002518	Pa×s	537.62	Joback Method
dvisc	0.0002152	Pa×s	574.42	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10103067&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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