

Naphthalene, 1,2,3,5,6-pentamethyl

Inchi:	InChI=1S/C15H18/c1-9-6-7-14-13(5)11(3)10(2)8-15(14)12(9)4/h6-8H,1-5H3
InchiKey:	OOJPMOFGUISHNV-UHFFFAOYSA-N
Formula:	C15H18
SMILES:	Cc1cc2c(C)c(C)ccc2c(C)c1C
Mol. weight [g/mol]:	198.30

Physical Properties

Property code	Value	Unit	Source
gf	246.33	kJ/mol	Joback Method
hf	17.32	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	56.21	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.382		Crippen Method
mcvol	178.990	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	316.28		NIST Webbook
rinpol	314.27		NIST Webbook
ripol	288.09		NIST Webbook
tb	613.16	K	Joback Method
tc	835.07	K	Joback Method
tf	380.53	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.97	J/molxK	613.16	Joback Method
cpg	454.18	J/molxK	650.14	Joback Method
cpg	469.48	J/molxK	687.13	Joback Method
cpg	483.90	J/molxK	724.11	Joback Method
cpg	497.51	J/molxK	761.10	Joback Method
cpg	510.34	J/molxK	798.08	Joback Method
cpg	522.44	J/molxK	835.07	Joback Method

dvisc	0.0008508	Paxs	380.53	Joback Method
dvisc	0.0006352	Paxs	419.30	Joback Method
dvisc	0.0004983	Paxs	458.07	Joback Method
dvisc	0.0004060	Paxs	496.85	Joback Method
dvisc	0.0003408	Paxs	535.62	Joback Method
dvisc	0.0002929	Paxs	574.39	Joback Method
dvisc	0.0002566	Paxs	613.16	Joback Method

Sources

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=R549145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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