

Naphthalene, 2-(1-methylethenyl)-

Other names:	2-(1-methylvinyl)naphthalene
Inchi:	InChI=1S/C13H12/c1-10(2)12-8-7-11-5-3-4-6-13(11)9-12/h3-9H,1H2,2H3
InchiKey:	ANCUXNXTHQXICN-UHFFFAOYSA-N
Formula:	C13H12
SMILES:	C=C(C)c1ccc2ccccc2c1
Mol. weight [g/mol]:	168.23
CAS:	3710-23-4

Physical Properties

Property code	Value	Unit	Source
gf	347.30	kJ/mol	Joback Method
hf	220.12	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	48.52	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.873		Crippen Method
mcvol	146.510	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	544.04	K	Joback Method
tc	779.75	K	Joback Method
tf	328.20 ± 2.00	K	NIST Webbook
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.83	J/mol×K	544.04	Joback Method
cpg	338.43	J/mol×K	583.32	Joback Method
cpg	352.85	J/mol×K	622.61	Joback Method
cpg	366.18	J/mol×K	661.89	Joback Method
cpg	378.51	J/mol×K	701.18	Joback Method
cpg	389.93	J/mol×K	740.46	Joback Method
cpg	400.53	J/mol×K	779.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3710234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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