

Naphthalene, (1-methylethyl)-

Other names:	isopropylnaphthalene
Inchi:	InChI=1S/C13H14/c1-10(2)12-9-5-7-11-6-3-4-8-13(11)12/h3-10H,1-2H3
InchiKey:	PMPBFICDXLLSRM-UHFFFAOYSA-N
Formula:	C13H14
SMILES:	CC(C)c1cccc2ccccc12
Mol. weight [g/mol]:	170.25
CAS:	29253-36-9

Physical Properties

Property code	Value	Unit	Source
gf	265.57	kJ/mol	Joback Method
hf	99.20	kJ/mol	Joback Method
hfus	16.57	kJ/mol	Joback Method
hvap	48.72	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.963		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	248.90		NIST Webbook
tb	541.30 ± 0.40	K	NIST Webbook
tc	778.34	K	Joback Method
tf	292.91	K	Joback Method
vc	0.572	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.66	J/mol×K	547.04	Joback Method
cpg	414.06	J/mol×K	739.79	Joback Method
cpg	401.80	J/mol×K	701.24	Joback Method
cpg	388.61	J/mol×K	662.69	Joback Method
cpg	374.41	J/mol×K	624.14	Joback Method
cpg	359.12	J/mol×K	585.59	Joback Method
cpg	425.45	J/mol×K	778.34	Joback Method

dvisc	0.0002758	Paxs	547.04	Joback Method
dvisc	0.0003344	Paxs	504.68	Joback Method
dvisc	0.0004201	Paxs	462.33	Joback Method
dvisc	0.0005526	Paxs	419.98	Joback Method
dvisc	0.0007731	Paxs	377.62	Joback Method
dvisc	0.0011772	Paxs	335.26	Joback Method
dvisc	0.0020244	Paxs	292.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29253369&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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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