Naphthalene, 1,2-dihydro-1,1,6-trimethyl-

Other names:	1,1,6-Trimethyl-1,2-dihydronaphthalene
	Dehydro-ar-ionene
	1,2-Dihydro-1,1,6-trimethylnaphthalene
	TDN
	1,1,6-trimethyl-1,2-dihydronaphthalene (TDN)
	1,1,6-Trimethyl-1,2-dihydro-naphthalene (dehydro-ar-ionene)
	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-, (TDN)
Inchi:	InChI=1S/C13H16/c1-10-6-7-12-11(9-10)5-4-8-13(12,2)3/h4-7,9H,8H2,1-3H3
InchiKey:	RTUMCNDCAVLXEP-UHFFFAOYSA-N
Formula:	C13H16
SMILES:	Cc1ccc2c(c1)C=CCC2(C)C
Mol. weight [g/mol]:	172.27
CAS:	30364-38-6

Physical Properties

Property code	Value	Unit	Source
gf	224.85	kJ/mol	Joback Method
hf	41.60	kJ/mol	Joback Method
hfus	13.65	kJ/mol	Joback Method
hvap	47.36	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.690		Crippen Method
mcvol	155.110	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1398.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1332.00		NIST Webbook

rinpol	1354.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1329.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1722.00		NIST Webbook
tb	543.89	K	Joback Method
tc	777.24	K	Joback Method
tf	326.81	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.55	J/mol×K	543.89	Joback Method
cpg	379.05	J/mol×K	582.78	Joback Method
cpg	395.29	J/mol×K	621.67	Joback Method
cpg	410.45	J/mol×K	660.56	Joback Method
cpg	424.69	J/mol×K	699.45	Joback Method
cpg	438.20	J/mol×K	738.35	Joback Method
cpg	451.14	J/mol×K	777.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30364386&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
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
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