Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-

Other names:	«alpha»-Ionene
	Ionene
	1,1,6-Trimethyl-1,2,3,4-tetrahydronaphthalene
	1,1,6-Trimethyltetralin
	1,2,3,4-Tetrahydro-1,1,6-trimethyl-naphthalene
	Naphthalene, tetrahydro-1,1,6-trimethyl-
	ionene (1,1,6-trimethyl-1,2,3,4-tetrahydronaphthalene)
Inchi:	InChI=1S/C13H18/c1-10-6-7-12-11(9-10)5-4-8-13(12,2)3/h6-7,9H,4-5,8H2,1-3H3
InchiKey:	LTMQZVLXCLQPCT-UHFFFAOYSA-N
Formula:	C13H18
SMILES:	Cc1ccc2c(c1)CCCC2(C)C
Mol. weight [g/mol]:	174.28
CAS:	475-03-6

Physical Properties

Property code	Value	Unit	Source
gf	194.89	kJ/mol	Joback Method
hf	-16.18	kJ/mol	Joback Method
hfus	12.43	kJ/mol	Joback Method
hvap	47.07	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.609		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1255.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1255.90		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1255.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1565.00		NIST Webbook
tb	544.73	K	Joback Method

tc	775.72	K	Joback Method
tf	326.05	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.21	J/mol×K	544.73	Joback Method
cpg	398.97	J/mol×K	583.23	Joback Method
cpg	416.43	J/mol×K	621.73	Joback Method
cpg	432.76	J/mol×K	660.23	Joback Method
cpg	448.14	J/mol×K	698.72	Joback Method
cpg	462.73	J/mol×K	737.22	Joback Method
cpg	476.69	J/mol×K	775.72	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	511.70	K	97.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C475036&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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