

Naphthalene, 1,2,4a,5,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)- [1S-(1«alpha»,4a«beta»,8a«alpha»)]-

Other names:	Cadina-3,9-diene «beta»-Cadinene, (-)- (-)-«beta»-Cadinene Cadine-3,9-diene NCI-C56008 1-Isopropyl-4,7-dimethyl-1,2,4a,5,8,8a-hexahydronaphthalene-, [1S-(1«alpha»,4a«beta»,8a«alpha»)]- «beta»-Cadinene beta-Cadinene Naphthalene, 1,2,4a,5,8,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S,4aR,8aS)- InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5-6,10,13-15H,7-9H2,1
Inchi:	
InchiKey:	USDOQCCMRDNVAH-RBSFLKMASA-N
Formula:	C15H24
SMILES:	CC1=CCC2C(C)=CCC(C(C)C)C2C1
Mol. weight [g/mol]:	204.35
CAS:	523-47-7

Physical Properties

Property code	Value	Unit	Source
gf	179.03	kJ/mol	Joback Method
hf	-164.97	kJ/mol	Joback Method
hfus	21.69	kJ/mol	Joback Method
hvap	50.71	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1491.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1523.00		NIST Webbook

rinpol	1518.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1523.00		NIST Webbook
ripol	1720.00		NIST Webbook
tb	576.33	K	Joback Method
tc	791.72	K	Joback Method
tf	287.93	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.29	J/mol×K	576.33	Joback Method
cpg	604.51	J/mol×K	755.83	Joback Method
cpg	586.71	J/mol×K	719.93	Joback Method
cpg	567.74	J/mol×K	684.03	Joback Method
cpg	547.54	J/mol×K	648.13	Joback Method
cpg	526.08	J/mol×K	612.23	Joback Method

cpg	621.19	J/mol×K	791.72	Joback Method
dvisc	0.0003401	Pa×s	576.33	Joback Method
dvisc	0.0004008	Pa×s	528.26	Joback Method
dvisc	0.0004882	Pa×s	480.20	Joback Method
dvisc	0.0006213	Pa×s	432.13	Joback Method
dvisc	0.0008398	Pa×s	384.06	Joback Method
dvisc	0.0012375	Pa×s	336.00	Joback Method
dvisc	0.0020754	Pa×s	287.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C523477&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

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
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

Latest version available from:

<https://www.chemeo.com/cid/42-895-2/Naphthalene-1-2-4a-5-8-8a-hexahydro-4-7-dimethyl-1-1-methylethyl-1S-1-alp>

Generated by Cheméo on 2025-12-05 14:08:29.119948481 +0000 UTC m=+4691906.649989145.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.