Cubenene

Other names:	Cadina-1,4-diene, cis
	Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-dimethyl-4-(1-methylethyl)-, [1S-(1«alpha»,4«alpha»,4a«alpha»)]-
	(1S,4S,4aR)-4-Isopropyl-1,6-dimethyl-1,2,3,4,4a,7-hexahydronaphthalene
	Cadina-1,4-diene
	4-Isopropyl-1,6-dimethyl-1,2,3,4,4a,7-hexahydronaphthalene-, [1S-(1«alpha»,4«alpha»,4a«alpha»)]-
	Cadina-1(2),4-diene
	Cadina-1,4-diene (= cubenene)
	cadina-1,4-diene (cubenene)
	Cadina-1,4-diene (=Cubinene)
Inchi:	InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h7,9-10,12-13,15H,5-6,8
InchiKey:	JUQGWBAOQUBVFP-DNOWBOINSA-N
Formula:	C15H24
SMILES:	CC1=CC2C(=CC1)C(C)CCC2C(C)C
Mol. weight [g/mol]:	204.35
CAS:	29837-12-5

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	1533.00		NIST Webbook
rinpol	1532.00		NIST Webbook
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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	526.08	J/mol×K	612.23	Joback Method
cpg	547.54	J/mol×K	648.13	Joback Method
cpg	567.74	J/mol×K	684.03	Joback Method
cpg	586.71	J/mol×K	719.93	Joback Method
cpg	604.51	J/mol×K	755.83	Joback Method
cpg	621.19	J/mol×K	791.72	Joback Method
dvisc	0.0020754	Pa×s	287.93	Joback Method
dvisc	0.0012375	Pa×s	336.00	Joback Method
dvisc	0.0008398	Pa×s	384.06	Joback Method
dvisc	0.0006213	Pa×s	432.13	Joback Method
dvisc	0.0004882	Pa×s	480.20	Joback Method
dvisc	0.0004008	Pa×s	528.26	Joback Method
dvisc	0.0003401	Pa×s	576.33	Joback Method

Sources

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McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29837125&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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