

Cadina-1,4-dien-3-ol

Other names:	Cadina-1,4-diene-3-ol
Inchi:	InChI=1S/C15H24O/c1-9(2)12-6-5-10(3)13-8-15(16)11(4)7-14(12)13/h7-10,12,14-16H,5-
InchiKey:	PDDMWQFBZZFOQR-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1=CC2C(=CC1O)C(C)CCC2C(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	34.50	kJ/mol	Joback Method
hf	-337.54	kJ/mol	Joback Method
hfus	26.85	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.552		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1656.00		NIST Webbook
tb	663.84	K	Joback Method
tc	864.81	K	Joback Method
tf	344.51	K	Joback Method
vc	0.741	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.38	J/mol×K	663.84	Joback Method
cpg	597.29	J/mol×K	697.34	Joback Method
cpg	615.12	J/mol×K	730.83	Joback Method

cpg	631.91	J/molxK	764.33	Joback Method
cpg	647.70	J/molxK	797.82	Joback Method
cpg	662.51	J/molxK	831.32	Joback Method
cpg	676.39	J/molxK	864.81	Joback Method
dvisc	0.0043769	Paxs	344.51	Joback Method
dvisc	0.0016494	Paxs	397.73	Joback Method
dvisc	0.0007826	Paxs	450.95	Joback Method
dvisc	0.0004346	Paxs	504.17	Joback Method
dvisc	0.0002700	Paxs	557.40	Joback Method
dvisc	0.0001823	Paxs	610.62	Joback Method
dvisc	0.0001311	Paxs	663.84	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R42045&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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