

Cadina-1, 3, 8-triene

Inchi:	InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5-8,10,12-13,15H,9H2,
InchiKey:	JQXHLPPXYMLHFB-NEJHNUGDSA-N
Formula:	C15H22
SMILES:	CC1=CC=C2C(C)C=CC(C(C)C)C2C1
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	208.99	kJ/mol	Joback Method
hf	-107.19	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hvap	51.00	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.357		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1565.00		NIST Webbook
tb	575.49	K	Joback Method
tc	792.92	K	Joback Method
tf	288.69	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.31	J/molxK	575.49	Joback Method
cpg	505.01	J/molxK	611.73	Joback Method
cpg	525.43	J/molxK	647.97	Joback Method
cpg	544.60	J/molxK	684.21	Joback Method
cpg	562.58	J/molxK	720.45	Joback Method
cpg	579.43	J/molxK	756.68	Joback Method
cpg	595.19	J/molxK	792.92	Joback Method
dvisc	0.0017701	Paxs	288.69	Joback Method
dvisc	0.0011118	Paxs	336.49	Joback Method

dvisc	0.0007840	Paxs	384.29	Joback Method
dvisc	0.0005973	Paxs	432.09	Joback Method
dvisc	0.0004804	Paxs	479.89	Joback Method
dvisc	0.0004019	Paxs	527.69	Joback Method
dvisc	0.0003464	Paxs	575.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R439682&Units=SI

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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