

10-«beta»(H)-Cadina-1(6),4-diene

Inchi:	InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h9-10,12-13H,5-8H2,1-4
InchiKey:	ULTBCADWJVQRCF-PZORYLMUSA-N
Formula:	C15H24
SMILES:	CC1=CC2=C(CC1)C(C)CCC2C(C)C
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	177.11	kJ/mol	Joback Method
hf	-156.10	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1474.00		NIST Webbook
tb	585.98	K	Joback Method
tc	802.43	K	Joback Method
tf	304.69	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.23	J/mol×K	585.98	Joback Method
cpg	525.21	J/mol×K	622.06	Joback Method
cpg	545.92	J/mol×K	658.13	Joback Method
cpg	565.40	J/mol×K	694.21	Joback Method
cpg	583.72	J/mol×K	730.28	Joback Method
cpg	600.91	J/mol×K	766.36	Joback Method

cpg	617.03	J/mol×K	802.43	Joback Method
dvisc	0.0020981	Pa×s	304.69	Joback Method
dvisc	0.0012209	Pa×s	351.57	Joback Method
dvisc	0.0008070	Pa×s	398.45	Joback Method
dvisc	0.0005820	Pa×s	445.34	Joback Method
dvisc	0.0004467	Pa×s	492.22	Joback Method
dvisc	0.0003590	Pa×s	539.10	Joback Method
dvisc	0.0002988	Pa×s	585.98	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=R587281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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