

1,4,9-cadalatriene

Inchi:	InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h6,11,14H,1,5,7-9H2,2-4
InchiKey:	AXSBOQMUBMOKDF-UHFFFAOYSA-N
Formula:	C15H22
SMILES:	C=C(C)C1=C2CC(C)CCC2C(C)=CC1
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	258.84	kJ/mol	Joback Method
hf	-35.18	kJ/mol	Joback Method
hfus	21.16	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.645		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1601.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
ripol	1962.00		NIST Webbook
ripol	1962.00		NIST Webbook
ripol	1962.00		NIST Webbook
tb	582.98	K	Joback Method
tc	803.24	K	Joback Method
tf	303.97	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.60	J/molxK	582.98	Joback Method
cpg	502.93	J/molxK	619.69	Joback Method
cpg	522.97	J/molxK	656.40	Joback Method
cpg	541.78	J/molxK	693.11	Joback Method

cpg	559.44	J/mol×K	729.82	Joback Method
cpg	575.99	J/mol×K	766.53	Joback Method
cpg	591.50	J/mol×K	803.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R238132&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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

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