

Cyclofarnesa-5(14),8,10-triene

Inchi:	InChI=1S/C15H24/c1-6-12(2)9-10-14-13(3)8-7-11-15(14,4)5/h6,9,14H,1,3,7-8,10-11H2,2
InchiKey:	IBRVHPJMXXNBAD-FMIVXFBMSA-N
Formula:	C15H24
SMILES:	<chem>C=CC(C)=CCC1C(=C)CCCC1(C)C</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	299.26	kJ/mol	Joback Method
hf	13.39	kJ/mol	Joback Method
hfus	17.67	kJ/mol	Joback Method
hvap	47.48	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinqol	1441.00		NIST Webbook
tb	557.60	K	Joback Method
tc	767.51	K	Joback Method
tf	278.73	K	Joback Method
vc	0.751	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.17	J/molxK	557.60	Joback Method
cpg	512.41	J/molxK	592.58	Joback Method
cpg	532.40	J/molxK	627.57	Joback Method
cpg	551.29	J/molxK	662.55	Joback Method
cpg	569.18	J/molxK	697.54	Joback Method
cpg	586.21	J/molxK	732.52	Joback Method
cpg	602.49	J/molxK	767.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R428058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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