

Bicyclohexyl-3,3'-diene

Inchi:	InChI=1S/C12H18/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-3,5,11-12H,4,6-10H2
InchiKey:	FRQGUZFWAVVQLA-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	C1=CCC(C2CC=CCC2)CC1
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	158.98	kJ/mol	Joback Method
hf	-66.81	kJ/mol	Joback Method
hfus	12.95	kJ/mol	Joback Method
hvap	43.75	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.699		Crippen Method
mcvol	149.620	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	1301.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1340.00		NIST Webbook
tb	511.38	K	Joback Method
tc	748.33	K	Joback Method
tf	241.28	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.94	J/molxK	511.38	Joback Method
cpg	452.85	J/molxK	708.84	Joback Method
cpg	435.17	J/molxK	669.35	Joback Method
cpg	416.09	J/molxK	629.85	Joback Method
cpg	395.57	J/molxK	590.36	Joback Method
cpg	373.54	J/molxK	550.87	Joback Method
cpg	469.20	J/molxK	748.33	Joback Method

dvisc	0.0002539	Paxs	511.38	Joback Method
dvisc	0.0003368	Paxs	466.36	Joback Method
dvisc	0.0004747	Paxs	421.35	Joback Method
dvisc	0.0007261	Paxs	376.33	Joback Method
dvisc	0.0012468	Paxs	331.31	Joback Method
dvisc	0.0025376	Paxs	286.30	Joback Method
dvisc	0.0067331	Paxs	241.28	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=R136353&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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