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: FRQGUZFVAWVQLA-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	1340.00		NIST Webbook
rinpol	1301.00		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/mol×K	511.38	Joback Method
cpg	373.54	J/mol×K	550.87	Joback Method
cpg	395.57	J/mol×K	590.36	Joback Method
cpg	416.09	J/mol×K	629.85	Joback Method
cpg	435.17	J/mol×K	669.35	Joback Method
cpg	452.85	J/mol×K	708.84	Joback Method
cpg	469.20	J/mol×K	748.33	Joback Method

dvisc	0.0067331	Pa×s	241.28	Joback Method
dvisc	0.0025376	Pa×s	286.30	Joback Method
dvisc	0.0012468	Pa×s	331.31	Joback Method
dvisc	0.0007261	Pa×s	376.33	Joback Method
dvisc	0.0004747	Pa×s	421.35	Joback Method
dvisc	0.0003368	Pa×s	466.36	Joback Method
dvisc	0.0002539	Pa×s	511.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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