

Bicyclohexyl-3-ene

Inchi:	InChI=1S/C12H20/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1,3,11-12H,2,4-10H2
InchiKey:	NHEQDCVKZARUJD-UHFFFAOYSA-N
Formula:	C12H20
SMILES:	C1=CCC(C2CCCCC2)CC1
Mol. weight [g/mol]:	164.29

Physical Properties

Property code	Value	Unit	Source
gf	129.02	kJ/mol	Joback Method
hf	-124.59	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	43.46	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.923		Crippen Method
mcvol	153.920	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1299.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1336.00		NIST Webbook
tb	512.22	K	Joback Method
tc	746.70	K	Joback Method
tf	240.52	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.46	J/molxK	512.22	Joback Method
cpg	392.31	J/molxK	551.30	Joback Method
cpg	415.56	J/molxK	590.38	Joback Method
cpg	437.28	J/molxK	629.46	Joback Method
cpg	457.51	J/molxK	668.54	Joback Method
cpg	476.31	J/molxK	707.62	Joback Method
cpg	493.75	J/molxK	746.70	Joback Method

dvisc	0.0085432	Paxs	240.52	Joback Method
dvisc	0.0029911	Paxs	285.80	Joback Method
dvisc	0.0013955	Paxs	331.09	Joback Method
dvisc	0.0007822	Paxs	376.37	Joback Method
dvisc	0.0004964	Paxs	421.65	Joback Method
dvisc	0.0003441	Paxs	466.94	Joback Method
dvisc	0.0002545	Paxs	512.22	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=R136368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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