

(Z)-Bicyclo[10.1.0]trideca-4,8-diene

Inchi:	InChI=1S/C13H20/c1-2-4-6-8-10-13-11-12(13)9-7-5-3-1/h3-6,12-13H,1-2,7-11H2/b5-3-,6
InchiKey:	OKQPAVLKCLUCOF-GLIMQPGKSA-N
Formula:	C13H20
SMILES:	C1=CCCC2CC2CCC=CCC1
Mol. weight [g/mol]:	176.30

Physical Properties

Property code	Value	Unit	Source
gf	155.30	kJ/mol	Joback Method
hf	-93.61	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	46.15	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.089		Crippen Method
mcvol	163.710	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinsol	1421.00		NIST Webbook
tb	538.53	K	Joback Method
tc	779.84	K	Joback Method
tf	249.03	K	Joback Method
vc	0.594	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.16	J/molxK	538.53	Joback Method
cpg	511.18	J/molxK	739.62	Joback Method
cpg	492.38	J/molxK	699.40	Joback Method
cpg	472.03	J/molxK	659.18	Joback Method
cpg	450.08	J/molxK	618.97	Joback Method
cpg	426.48	J/molxK	578.75	Joback Method
cpg	528.50	J/molxK	779.84	Joback Method
dvisc	0.0001897	Paxs	538.53	Joback Method
dvisc	0.0002638	Paxs	490.28	Joback Method

dvisc	0.0003942	Paxs	442.03	Joback Method
dvisc	0.0006502	Paxs	393.78	Joback Method
dvisc	0.0012331	Paxs	345.53	Joback Method
dvisc	0.0028788	Paxs	297.28	Joback Method
dvisc	0.0093345	Paxs	249.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R2914&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
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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