

Bicyclo[5.3.1]undeca-1,3,5,7,9-pentaene

Inchi:	InChI=1S/C11H10/c1-2-5-10-7-4-8-11(9-10)6-3-1/h1-8H,9H2/b2-1-,3-1-,5-2-,6-3-,10-5-,1
InchiKey:	PVDVWMOTLDWVRK-FLXUIKBISA-N
Formula:	C11H10
SMILES:	C1=CC=C2C=CC=C(C=C1)C2
Mol. weight [g/mol]:	142.20
CAS:	65754-71-4

Physical Properties

Property code	Value	Unit	Source
gf	248.70	kJ/mol	Joback Method
hf	400.00	kJ/mol	NIST Webbook
hfus	13.21	kJ/mol	Joback Method
hvap	44.17	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.925		Crippen Method
mcvol	122.630	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	501.01	K	Joback Method
tc	743.67	K	Joback Method
tf	269.33	K	Joback Method
vc	0.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.65	J/molxK	501.01	Joback Method
cpg	267.47	J/molxK	541.45	Joback Method
cpg	282.05	J/molxK	581.90	Joback Method
cpg	295.48	J/molxK	622.34	Joback Method
cpg	307.83	J/molxK	662.79	Joback Method
cpg	319.18	J/molxK	703.23	Joback Method
cpg	329.61	J/molxK	743.67	Joback Method
dvisc	0.0024177	Paxs	269.33	Joback Method
dvisc	0.0013227	Paxs	307.94	Joback Method

dvisc	0.0008278	Paxs	346.56	Joback Method
dvisc	0.0005691	Paxs	385.17	Joback Method
dvisc	0.0004189	Paxs	423.78	Joback Method
dvisc	0.0003245	Paxs	462.40	Joback Method
dvisc	0.0002615	Paxs	501.01	Joback Method

Sources

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=C65754714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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