

Bicyclo[5.4.2]trideca-7,9,11,12-tetraene

Inchi:	InChI=1S/C13H16/c1-2-6-12-8-4-5-9-13(7-3-1)11-10-12/h4-5,8-11H,1-3,6-7H2/b5-4-,8-4-
InchiKey:	XRWAKCPFJMTBC-VBKZNOIUSA-N
Formula:	C13H16
SMILES:	C1=CC=C2C=CC(=C1)CCCC2
Mol. weight [g/mol]:	172.27
CAS:	33800-90-7

Physical Properties

Property code	Value	Unit	Source
gf	211.38	kJ/mol	Joback Method
hf	39.69	kJ/mol	Joback Method
hfus	12.96	kJ/mol	Joback Method
hvap	48.67	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
log10ws	-4.47		Crippen Method
logp	3.929		Crippen Method
mcvol	155.110	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
tb	556.15	K	Joback Method
tc	804.85	K	Joback Method
tf	284.07	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.40	J/molxK	556.15	Joback Method
cpg	384.26	J/molxK	597.60	Joback Method
cpg	403.58	J/molxK	639.05	Joback Method
cpg	421.45	J/molxK	680.50	Joback Method
cpg	437.92	J/molxK	721.95	Joback Method
cpg	453.06	J/molxK	763.40	Joback Method
cpg	466.94	J/molxK	804.85	Joback Method
dvisc	0.0046615	Paxs	284.07	Joback Method

dvisc	0.0017632	Paxs	329.42	Joback Method
dvisc	0.0008438	Paxs	374.76	Joback Method
dvisc	0.0004735	Paxs	420.11	Joback Method
dvisc	0.0002973	Paxs	465.46	Joback Method
dvisc	0.0002028	Paxs	510.80	Joback Method
dvisc	0.0001472	Paxs	556.15	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=C33800907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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