

10,18-Bisnorabieta-5,7,9(10),11,13-pentaene

Inchi:	InChI=1S/C18H22/c1-12(2)14-7-10-17-15(11-14)8-9-16-13(3)5-4-6-18(16)17/h7-13H,4-6H
InchiKey:	PEGDXOHRNDHEEB-UHFFFAOYSA-N
Formula:	C18H22
SMILES:	CC(C)c1ccc2c3c(ccc2c1)C(C)CCC3
Mol. weight [g/mol]:	238.37
CAS:	6566-19-4

Physical Properties

Property code	Value	Unit	Source
gf	337.06	kJ/mol	Joback Method
hf	39.70	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.403		Crippen Method
mcvol	210.400	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2082.00		NIST Webbook
tb	682.41	K	Joback Method
tc	916.74	K	Joback Method
tf	388.72	K	Joback Method
vc	0.800	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.52	J/molxK	682.41	Joback Method
cpg	603.28	J/molxK	721.46	Joback Method
cpg	621.70	J/molxK	760.52	Joback Method
cpg	638.87	J/molxK	799.57	Joback Method
cpg	654.92	J/molxK	838.63	Joback Method
cpg	669.94	J/molxK	877.68	Joback Method
cpg	684.05	J/molxK	916.74	Joback Method
dvisc	0.0016811	Paxs	388.72	Joback Method

dvisc	0.0011490	Paxs	437.67	Joback Method
dvisc	0.0008478	Paxs	486.62	Joback Method
dvisc	0.0006613	Paxs	535.57	Joback Method
dvisc	0.0005377	Paxs	584.51	Joback Method
dvisc	0.0004515	Paxs	633.46	Joback Method
dvisc	0.0003887	Paxs	682.41	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6566194&Units=SI

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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