BICYCLO[4.4.1]UNDECA-1,3,5,7,9-PENTAENE

Other names: 1,6-Methano[10]annulene
Inchi: InChI=1S/C11H10/c1-2-6-11-8-4-3-7-10(5-1)9-11/h1-8H,9H2
InchiKey: OORRQYZWSVJKSO-UHFFFAOYSA-N
Formula: C11H10
SMILES: C1=CC=C2C=CC=CC(=C1)C2
Mol. weight [g/mol]: 142.20

Physical Properties

Property code	Value	Unit	Source
chl	-6011.99	kJ/mol	NIST Webbook
hf	315.00 ± 3.00	kJ/mol	NIST Webbook
hf	323.00	kJ/mol	NIST Webbook
hfl	254.00 ± 2.00	kJ/mol	NIST Webbook
hfus	13.21	kJ/mol	Joback Method
hvap	60.75	kJ/mol	NIST Webbook
hvap	61.00	kJ/mol	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.92	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
logp	2.925		Crippen Method
mcvol	122.630	ml/mol	McGowan Method
tf	301.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.65	J/mol×K	501.01	Joback Method
cpg	267.47	J/mol×K	541.45	Joback Method
cpg	282.05	J/mol×K	581.90	Joback Method
cpg	295.48	J/mol×K	622.34	Joback Method
cpg	307.83	J/mol×K	662.79	Joback Method
cpg	319.18	J/mol×K	703.23	Joback Method
cpg	329.61	J/mol×K	743.67	Joback Method
dvisc	0.0024177	Pa×s	269.33	Joback Method

dvisc	0.0013227	Pa×s	307.94	Joback Method
dvisc	0.0008278	Pa×s	346.56	Joback Method
dvisc	0.0005691	Pa×s	385.17	Joback Method
dvisc	0.0004189	Pa×s	423.78	Joback Method
dvisc	0.0003245	Pa×s	462.40	Joback Method
dvisc	0.0002615	Pa×s	501.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.00 ± 2.00	K	0.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2443461&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point