11-Azabicyclo[4.4.1]undeca-1,3,5,7,9-pentaene

Other names: 1,6-Imino-(10)annulene
Inchi: InChI=1S/C10H9N/c1-2-6-10-8-4-3-7-9(5-1)11-10/h1-8,11H
InchiKey: DJDJGVOVSUVRDI-UHFFFAOYSA-N
Formula: C10H9N
SMILES: C1=CC=C2C=CC=CC(=C1)N2
Mol. weight [g/mol]: 143.19
CAS: 4753-55-3

Physical Properties

Property code	Value	Unit	Source
chl	-5529.24	kJ/mol	NIST Webbook
gf	327.99	kJ/mol	Joback Method
hf	367.00 ± 3.00	kJ/mol	NIST Webbook
hfl	308.00 ± 3.00	kJ/mol	NIST Webbook
hfus	20.21	kJ/mol	Joback Method
hvap	59.00	kJ/mol	NIST Webbook
hvap	59.29	kJ/mol	NIST Webbook
ie	7.75	eV	NIST Webbook
ie	8.01	eV	NIST Webbook
log10ws	-3.25		Crippen Method
logp	2.040		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	526.68	K	Joback Method
tc	779.16	K	Joback Method
tf	289.00	K	NIST Webbook
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.93	J/mol×K	526.68	Joback Method
cpg	262.58	J/mol×K	568.76	Joback Method
cpg	276.09	J/mol×K	610.84	Joback Method

cpg	288.52	J/mol×K	652.92	Joback Method
cpg	299.95	J/mol×K	695.00	Joback Method
cpg	310.43	J/mol×K	737.08	Joback Method
cpg	320.05	J/mol×K	779.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.50 ± 0.50	K	0.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4753553&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume