Bicyclo[4.4.1]undeca-1,3,5,8-tetralene

Inchi: InChI=1S/C11H12/c1-2-6-11-8-4-3-7-10(5-1)9-11/h1-8,10-11H,9H2
InchiKey: ZVYFTKULEILVHY-UHFFFAOYSA-N
Formula: C11H12
SMILES: C1=CC2C=CC=CC(C=C1)C2
Mol. weight [g/mol]: 144.21
CAS: 6074-99-3

Physical Properties

Property code	Value	Unit	Source
chl	-6230.00 ± 30.00	kJ/mol	NIST Webbook
gf	222.58	kJ/mol	Joback Method
hf	261.00	kJ/mol	NIST Webbook
hfus	14.90	kJ/mol	Joback Method
hvap	41.93	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.861		Crippen Method
mcvol	126.930	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	482.55	K	Joback Method
tc	719.69	K	Joback Method
tf	235.05	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.78	J/mol×K	482.55	Joback Method
cpg	287.89	J/mol×K	522.07	Joback Method
cpg	305.63	J/mol×K	561.60	Joback Method
cpg	322.05	J/mol×K	601.12	Joback Method
cpg	337.24	J/mol×K	640.64	Joback Method
cpg	351.25	J/mol×K	680.16	Joback Method
cpg	364.16	J/mol×K	719.69	Joback Method
dvisc	0.0027522	Pa×s	235.05	Joback Method

dvisc	0.0014598	Pa×s	276.30	Joback Method
dvisc	0.0009129	Pa×s	317.55	Joback Method
dvisc	0.0006360	Pa×s	358.80	Joback Method
dvisc	0.0004774	Pa×s	400.05	Joback Method
dvisc	0.0003781	Pa×s	441.30	Joback Method
dvisc	0.0003116	Pa×s	482.55	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=C6074993&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume