[18]-Annulene

Other names: (1,3,5,7,9,11,13,15,17)-Cyclooctadecanonaene
Inchi: InChI=1S/C18H18/c1-2-4-6-8-10-12-14-16-18-17-15-13-11-9-7-5-3-1/h1-18H/b2-1-,3-1+,
InchiKey: STQWAGYDANTDNA-DWSNDWDZSA-N
Formula: C18H18
SMILES: c1ccccccccccccccccc1
Mol. weight [g/mol]: 234.34
CAS: 2040-73-5

Physical Properties

Property code	Value	Unit	Source
chs	-9819.00 ± 17.00	kJ/mol	NIST Webbook
gf	257.28	kJ/mol	Joback Method
hf	280.00 ± 25.00	kJ/mol	NIST Webbook
hfs	163.00 ± 17.00	kJ/mol	NIST Webbook
hfus	18.94	kJ/mol	Joback Method
hsub	120.00 ± 8.00	kJ/mol	NIST Webbook
hsub	117.00	kJ/mol	NIST Webbook
hvap	61.09	kJ/mol	Joback Method
ie	6.60	eV	NIST Webbook
ie	7.23	eV	NIST Webbook
log10ws	-4.98		Crippen Method
logp	5.060		Crippen Method
mcvol	214.920	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
tb	679.14	K	Joback Method
tc	963.80	K	Joback Method
tf	268.84	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.78	J/mol×K	679.14	Joback Method
cpg	647.94	J/mol×K	916.36	Joback Method

cpg	633.67	J/mol×K	868.91	Joback Method
cpg	616.57	J/mol×K	821.47	Joback Method
cpg	596.69	J/mol×K	774.03	Joback Method
cpg	574.07	J/mol×K	726.58	Joback Method
cpg	659.32	J/mol×K	963.80	Joback Method
dvisc	0.0000042	Pa×s	679.14	Joback Method
dvisc	0.0000082	Pa×s	610.76	Joback Method
dvisc	0.0000191	Pa×s	542.37	Joback Method
dvisc	0.0000565	Pa×s	473.99	Joback Method
dvisc	0.0002406	Pa×s	405.61	Joback Method
dvisc	0.0018462	Pa×s	337.22	Joback Method
dvisc	0.0399459	Pa×s	268.84	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2040735&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

chs: Standard solid 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
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume