Pentacyclo[18.2.2.2(9,12).0(4,15).0(6,17)]hexacosa

Inchi: InChI=1S/C26H26/c1-2-21-10-14-25-17-24-13-9-20-6-4-19(5-7-20)8-12-23(25)18-26(24)
InchiKey: REXZNBNRGIQZSK-UHFFFAOYSA-N
Formula: C26H26
SMILES: c1cc2cc(c1)CCc1cc3c(cc1CCc1ccc(cc1)CC3)CC2
Mol. weight [g/mol]: 338.48
CAS: 35117-21-6

Physical Properties

Property code	Value	Unit	Source
chs	-14230.90 ± 3.60	kJ/mol	NIST Webbook
gf	569.84	kJ/mol	Joback Method
hf	409.70 ± 5.60	kJ/mol	NIST Webbook
hfs	283.80 ± 5.00	kJ/mol	NIST Webbook
hfus	33.20	kJ/mol	Joback Method
hsub	125.90 ± 2.50	kJ/mol	NIST Webbook
hsub	125.90	kJ/mol	NIST Webbook
hvap	84.40	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	5.454		Crippen Method
mcvol	284.200	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	930.58	K	Joback Method
tc	1201.79	K	Joback Method
tf	561.96	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.79	J/mol×K	1156.59	Joback Method
cpg	1012.28	J/mol×K	1201.79	Joback Method
cpg	910.64	J/mol×K	930.58	Joback Method
cpg	929.86	J/mol×K	975.78	Joback Method
cpg	947.84	J/mol×K	1020.98	Joback Method

cpg	964.82	J/mol×K	1066.18	Joback Method
cpg	981.06	J/mol×K	1111.39	Joback Method
dvisc	0.0001498	Pa×s	930.58	Joback Method
dvisc	0.0001810	Pa×s	869.14	Joback Method
dvisc	0.0008681	Pa×s	561.96	Joback Method
dvisc	0.0005606	Pa×s	623.40	Joback Method
dvisc	0.0003916	Pa×s	684.83	Joback Method
dvisc	0.0002902	Pa×s	746.27	Joback Method
dvisc	0.0002251	Pa×s	807.71	Joback Method
hsubt	119.10 ± 1.50	kJ/mol	355.50	NIST Webbook
hsubt	125.90 ± 2.50	kJ/mol	405.70	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35117216&Units=SI

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
hsubt: Enthalpy of sublimation at a given temperature
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