9,9'-BIPHENANTHRENE

Other names: 9,9'-Biphenanthryl
Inchi: InChI=1S/C28H18/c1-3-11-21-19(9-1)17-27(25-15-7-5-13-23(21)25)28-18-20-10-2-4-12-
InchiKey: UPAPZXUZBAAZCB-UHFFFAOYSA-N
Formula: C28H18
SMILES: c1ccc2c(c1)cc(-c1cc3ccccc3c3ccccc13)c1ccccc12
Mol. weight [g/mol]: 354.45

Physical Properties

Property code	Value	Unit	Source
af	0.6868		Cheméo Relay (1.0)
chs	-13804.20 ± 2.80	kJ/mol	NIST Webbook
gf	797.78	kJ/mol	Joback Method
hf	364.00	kJ/mol	NIST Webbook
hfs	212.80 ± 4.70	kJ/mol	NIST Webbook
hfus	42.88	kJ/mol	Joback Method
hsub	151.50	kJ/mol	NIST Webbook
hvap	163.02	kJ/mol	Cheméo Relay (1.0)
ie	7.34	eV	Cheméo Relay (1.0)
log10ws	-10.15		Cheméo Relay (1.0)
logp	7.966		Crippen Method
mcvol	280.020	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
tb	861.17	K	Cheméo Relay (1.0)
tc	1215.34	K	Cheméo Relay (1.0)
tf	534.50	K	Cheméo Relay (1.0)
vc	1.053	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.59	J/mol×K	989.24	Joback Method
cpg	864.57	J/mol×K	1035.75	Joback Method
cpg	881.61	J/mol×K	1082.26	Joback Method
cpg	899.10	J/mol×K	1128.76	Joback Method

cpg	917.37	J/mol×K	1175.27	Joback Method
cpg	936.81	J/mol×K	1221.78	Joback Method
cpg	957.76	J/mol×K	1268.29	Joback Method
dvisc	0.0018094	Pa×s	639.04	Joback Method
dvisc	0.0014638	Pa×s	697.41	Joback Method
dvisc	0.0012236	Pa×s	755.77	Joback Method
dvisc	0.0010495	Pa×s	814.14	Joback Method
dvisc	0.0009188	Pa×s	872.51	Joback Method
dvisc	0.0008179	Pa×s	930.87	Joback Method
dvisc	0.0007382	Pa×s	989.24	Joback Method
hsubt	151.00	kJ/mol	293.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20532030&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

Legend

af: Acentric Factor
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
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