DIBENZO[A,L]PENTACENE

Other names:	1,2,8,9-Dibenzpentacene
	1,2:8,9-Dibenzopentacene
	Dibenzo-1,2,8,9-pentacene
	1,2,8,9-Dibenzopentacene
	1,2:8,9-Dibenzpentacene
	Dibenzo(a1)pentacene
Inchi:	InChI=1S/C30H18/c1-3-7-27-19(5-1)9-11-21-13-23-16-26-18-30-22(12-10-20-6-2-4-8-28(
InchiKey:	XSTMLGGLUNLJRY-UHFFFAOYSA-N
Formula:	C30H18
SMILES:	c1ccc2c(c1)ccc1cc3cc4cc5c(ccc6ccccc65)cc4cc3cc12
Mol. weight [g/mol]:	378.47

Physical Properties

Property code	Value	Unit	Source
af	0.7634		Cheméo Relay (1.0)
gf	905.88	kJ/mol	Joback Method
hf	477.13	kJ/mol	Cheméo Relay (1.0)
hfus	47.67	kJ/mol	Joback Method
hvap	181.43	kJ/mol	Cheméo Relay (1.0)
ie	6.64 ± 0.02	eV	NIST Webbook
ie	6.42	eV	NIST Webbook
ie	6.77	eV	NIST Webbook
ie	7.00 ± 0.10	eV	NIST Webbook
ie	6.77	eV	NIST Webbook
log10ws	-11.93		Cheméo Relay (1.0)
logp	8.606		Crippen Method
mcvol	293.040	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
tb	939.73	K	Cheméo Relay (1.0)
tc	1300.36	K	Cheméo Relay (1.0)
tf	640.96	K	Cheméo Relay (1.0)
vc	1.116	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.76	J/mol×K	1051.26	Joback Method
cpg	929.78	J/mol×K	1097.80	Joback Method
cpg	951.06	J/mol×K	1144.33	Joback Method
cpg	974.05	J/mol×K	1190.87	Joback Method
cpg	999.18	J/mol×K	1237.40	Joback Method
cpg	1026.90	J/mol×K	1283.94	Joback Method
cpg	1057.66	J/mol×K	1330.47	Joback Method
dvisc	0.0046199	Pa×s	713.08	Joback Method
dvisc	0.0041148	Pa×s	769.44	Joback Method
dvisc	0.0037234	Pa×s	825.81	Joback Method
dvisc	0.0034125	Pa×s	882.17	Joback Method
dvisc	0.0031604	Pa×s	938.53	Joback Method
dvisc	0.0029526	Pa×s	994.90	Joback Method
dvisc	0.0027786	Pa×s	1051.26	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C227098&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
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