DIBENZ[A,J]ANTHRACENE

Other names: 1,2,7,8-dibenzanthracene
1,2:7,8-Dibenzanthracene
3,4,5,6-Dibenzanthracene
Dibenzo(a,j)anthracene
Dibenzo-1,2,7,8-anthracene
Inchi: InChI=1S/C22H14/c1-3-7-19-15(5-1)9-11-17-13-18-12-10-16-6-2-4-8-20(16)22(18)14-21(
InchiKey: KLIHYVJAYWCEDM-UHFFFAOYSA-N
Formula: C22H14
SMILES: c1ccc2c(c1)ccc1cc3ccc4ccccc4c3cc12
Mol. weight [g/mol]: 278.35

Physical Properties

Property code	Value	Unit	Source
af	0.6031		Cheméo Relay (1.0)
gf	644.48	kJ/mol	Joback Method
hf	355.38	kJ/mol	Cheméo Relay (1.0)
hfus	33.69	kJ/mol	Joback Method
hvap	128.72	kJ/mol	Cheméo Relay (1.0)
ie	7.15	eV	Cheméo Relay (1.0)
log10ws	-8.57		Cheméo Relay (1.0)
logp	6.299		Crippen Method
mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
tb	795.32	K	Cheméo Relay (1.0)
tc	1097.81	K	Cheméo Relay (1.0)
tf	519.57	K	Cheméo Relay (1.0)
vc	0.837	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.64	J/mol×K	820.30	Joback Method
cpg	622.45	J/mol×K	865.23	Joback Method
cpg	636.52	J/mol×K	910.16	Joback Method

cpg	650.13	J/mol×K	955.09	Joback Method
cpg	663.56	J/mol×K	1000.03	Joback Method
cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	691.04	J/mol×K	1089.89	Joback Method
dvisc	0.0022584	Pa×s	532.48	Joback Method
dvisc	0.0019125	Pa×s	580.45	Joback Method
dvisc	0.0016611	Pa×s	628.42	Joback Method
dvisc	0.0014719	Pa×s	676.39	Joback Method
dvisc	0.0013254	Pa×s	724.36	Joback Method
dvisc	0.0012090	Pa×s	772.33	Joback Method
dvisc	0.0011148	Pa×s	820.30	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C224419&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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