Dibenzo[cd,k]naphtho[3,2,1,8-pqra]perylene

Inchi: InChI=1S/C32H16/c1-2-8-21-18(5-1)16-26-25-13-11-17-6-3-9-22-23-10-4-7-19-15-20-12-
InchiKey: CPXFAEJNAVYPCD-UHFFFAOYSA-N
Formula: C32H16
SMILES: c1ccc2c(c1)cc1c3ccc4cccc5c6cccc7cc8ccc2c1c8c(c76)c3c45
Mol. weight [g/mol]: 400.47
CAS: 120836-02-4

Physical Properties

Property code	Value	Unit	Source
gf	1099.48	kJ/mol	Joback Method
hf	844.61	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	104.95	kJ/mol	Joback Method
log10ws	-14.15		Crippen Method
logp	9.226		Crippen Method
mcvol	295.200	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
tb	1121.84	K	Joback Method
tc	1399.15	K	Joback Method
tf	844.90	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.39	J/mol×K	1121.84	Joback Method
cpg	1152.95	J/mol×K	1352.93	Joback Method
cpg	1102.53	J/mol×K	1306.71	Joback Method
cpg	1057.97	J/mol×K	1260.50	Joback Method
cpg	1018.68	J/mol×K	1214.28	Joback Method
cpg	984.02	J/mol×K	1168.06	Joback Method
cpg	1209.85	J/mol×K	1399.15	Joback Method
dvisc	0.1126083	Pa×s	1121.84	Joback Method
dvisc	0.1110035	Pa×s	1075.68	Joback Method

dvisc	0.1092809	Pa×s	1029.53	Joback Method
dvisc	0.1074272	Pa×s	983.37	Joback Method
dvisc	0.1054271	Pa×s	937.21	Joback Method
dvisc	0.1032630	Pa×s	891.06	Joback Method
dvisc	0.1009143	Pa×s	844.90	Joback Method

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=C120836024&Units=SI

Legend

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
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