5,6-Dimethylchrysene

Inchi: InChI=1S/C20H16/c1-13-14(2)20-17-9-4-3-7-15(17)11-12-19(20)18-10-6-5-8-16(13)18/h3
InchiKey: SDOJHDGZFOGOFD-UHFFFAOYSA-N
Formula: C20H16
SMILES: Cc1c(C)c2c3ccccc3ccc2c2ccccc12
Mol. weight [g/mol]: 256.35

Physical Properties

Property code	Value	Unit	Source
gf	511.36	kJ/mol	Joback Method
hf	307.73	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	69.96	kJ/mol	Joback Method
log10ws	-7.01		Estimated Solubility Method
log10ws	-7.01		Aqueous Solubility Prediction Method
logp	5.763		Crippen Method
mcvol	210.520	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
tb	760.54	K	Joback Method
tc	1013.66	K	Joback Method
tf	402.45	K	Aqueous Solubility Prediction Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.63	J/mol×K	760.54	Joback Method
cpg	586.13	J/mol×K	802.73	Joback Method
cpg	600.62	J/mol×K	844.91	Joback Method
cpg	614.28	J/mol×K	887.10	Joback Method
cpg	627.28	J/mol×K	929.28	Joback Method
cpg	639.81	J/mol×K	971.47	Joback Method
cpg	652.05	J/mol×K	1013.66	Joback Method

dvisc	0.0014862	Pa×s	489.76	Joback Method
dvisc	0.0012234	Pa×s	534.89	Joback Method
dvisc	0.0010381	Pa×s	580.02	Joback Method
dvisc	0.0009019	Pa×s	625.15	Joback Method
dvisc	0.0007987	Pa×s	670.28	Joback Method
dvisc	0.0007181	Pa×s	715.41	Joback Method
dvisc	0.0006539	Pa×s	760.54	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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