8,12-Dimethylbenz[a]anthracene

Other names: 5,9-Dimethyl-1,2-benzanthracene
8,12-Dimethylbenz(a)anthracene
Inchi: InChI=1S/C20H16/c1-13-6-5-9-17-14(2)20-16(12-19(13)17)11-10-15-7-3-4-8-18(15)20/h3
InchiKey: FBIFSZUQMIZITB-UHFFFAOYSA-N
Formula: C20H16
SMILES: Cc1cccc2c(C)c3c(ccc4ccccc43)cc12
Mol. weight [g/mol]: 256.35

Physical Properties

Property code	Value	Unit	Source
af	0.5809		Cheméo Relay (1.0)
gf	511.36	kJ/mol	Joback Method
hf	241.13	kJ/mol	Cheméo Relay (1.0)
hfus	31.10	kJ/mol	Joback Method
hvap	113.49	kJ/mol	Cheméo Relay (1.0)
ie	7.11	eV	Cheméo Relay (1.0)
log10ws	-7.37		Cheméo Relay (1.0)
logp	5.763		Crippen Method
mcvol	210.520	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
tb	724.14	K	Cheméo Relay (1.0)
tc	1006.85	K	Cheméo Relay (1.0)
tf	407.68	K	Cheméo Relay (1.0)
vc	0.794	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20627310&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
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