

4H-Dibenz[a,k]anthracene

Inchi:	InChI=1S/C21H14/c1-2-9-18-14(5-1)11-12-17-13-16-8-3-6-15-7-4-10-19(20(15)16)21(17)
InchiKey:	NUXRXCMDYFQYEQ-UHFFFAOYSA-N
Formula:	C21H14
SMILES:	C1=Cc2cc3ccc4ccccc4c3c3cccc(c23)C1
Mol. weight [g/mol]:	266.34
CAS:	194-85-4

Physical Properties

Property code	Value	Unit	Source
gf	618.20	kJ/mol	Joback Method
hf	438.01	kJ/mol	Joback Method
hfus	31.97	kJ/mol	Joback Method
hvap	72.70	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	5.716		Crippen Method
mcvol	209.450	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
tb	793.99	K	Joback Method
tc	1059.55	K	Joback Method
tf	411.40 ± 2.00	K	NIST Webbook
vc	0.814	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.34	J/mol×K	793.99	Joback Method
cpg	646.11	J/mol×K	1015.29	Joback Method
cpg	632.78	J/mol×K	971.03	Joback Method
cpg	619.52	J/mol×K	926.77	Joback Method
cpg	606.05	J/mol×K	882.51	Joback Method
cpg	592.08	J/mol×K	838.25	Joback Method
cpg	659.79	J/mol×K	1059.55	Joback Method
dvisc	0.0015639	Paxs	793.99	Joback Method
dvisc	0.0016690	Paxs	748.99	Joback Method

dvisc	0.0017960	Paxs	703.98	Joback Method
dvisc	0.0019522	Paxs	658.98	Joback Method
dvisc	0.0021481	Paxs	613.98	Joback Method
dvisc	0.0023996	Paxs	568.97	Joback Method
dvisc	0.0027321	Paxs	523.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C194854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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