

3,9-Dimethylbenz[a]anthracene

Other names:	Benz(a)anthracene, 3,9-dimethyl-
Inchi:	InChI=1S/C20H16/c1-13-3-5-15-12-20-17(11-18(15)10-13)7-6-16-9-14(2)4-8-19(16)20/h
InchiKey:	DBPDWIZRMPUWRH-UHFFFAOYSA-N
Formula:	C20H16
SMILES:	<chem>Cc1ccc2cc3c(ccc4cc(C)ccc43)cc2c1</chem>
Mol. weight [g/mol]:	256.34
CAS:	316-51-8

Physical Properties

Property code	Value	Unit	Source
chs	-10233.00 ± 2.00	kJ/mol	NIST Webbook
gf	511.36	kJ/mol	Joback Method
hf	189.00 ± 3.00	kJ/mol	NIST Webbook
hf	189.10	kJ/mol	NIST Webbook
hfs	76.10 ± 2.80	kJ/mol	NIST Webbook
hfs	76.00 ± 3.00	kJ/mol	NIST Webbook
hfus	31.10	kJ/mol	Joback Method
hsub	113.00	kJ/mol	NIST Webbook
hsub	113.00 ± 2.00	kJ/mol	NIST Webbook
hvap	69.96	kJ/mol	Joback Method
ie	7.20 ± 0.03	eV	NIST Webbook
log10ws	-7.84		Crippen 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	489.76	K	Joback Method
vc	0.814	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.63	J/mol×K	760.54	Joback Method

cpg	639.81	J/molxK	971.47	Joback Method
cpg	627.28	J/molxK	929.28	Joback Method
cpg	614.28	J/molxK	887.10	Joback Method
cpg	600.62	J/molxK	844.91	Joback Method
cpg	586.13	J/molxK	802.73	Joback Method
cpg	652.05	J/molxK	1013.66	Joback Method
dvisc	0.0006539	Paxs	760.54	Joback Method
dvisc	0.0007181	Paxs	715.41	Joback Method
dvisc	0.0007987	Paxs	670.28	Joback Method
dvisc	0.0009019	Paxs	625.15	Joback Method
dvisc	0.0010381	Paxs	580.02	Joback Method
dvisc	0.0012234	Paxs	534.89	Joback Method
dvisc	0.0014862	Paxs	489.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C316518&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

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