3-Methylcholanthrene

Other names:	1,2-Dihydro-3-methylbenz[j]aceanthrylene
	20-MC
	20-Methylcholanthrene
	3-MC
	3-MCA
	3-Methylcholanthrene-(20)
	56-49-5
	Benz[j]aceanthrylene, 1,2-dihydro-3-methyl-
	Cholanthrene, 20(3)-methyl
	Cholanthrene, 3-methyl-
	MC
	MCA
	Methylcholanthrene
	NSC 21970
	Rcra waste number U157
Inchi:	InChI=1S/C21H16/c1-13-6-7-15-12-20-17-5-3-2-4-14(17)8-9-18(20)19-11-10-16(13)21(15
InchiKey:	PPQNQXQZIWHJRB-UHFFFAOYSA-N
Formula:	C21H16
SMILES:	Cc1ccc2cc3c(ccc4ccccc43)c3c2c1CC3
Mol. weight [g/mol]:	268.35
CAS:	56-49-5

Physical Properties

Property code	Value	Unit	Source
gf	590.71	kJ/mol	Joback Method
hf	374.92	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
ie	7.66	eV	NIST Webbook
log10ws	-7.97		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-7.94		Aqueous Solubility Prediction Method
logp	5.553		Crippen Method
mcvol	213.750	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	468.88		NIST Webbook

rinpol	2906.00		NIST Webbook
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook
rinpol	2911.00		NIST Webbook
rinpol	2900.00		NIST Webbook
rinpol	2906.00		NIST Webbook
rinpol	2906.00		NIST Webbook
rinpol	2877.00		NIST Webbook
rinpol	2906.00		NIST Webbook
rinpol	2959.00		NIST Webbook
rinpol	468.90		NIST Webbook
rinpol	467.70		NIST Webbook
rinpol	457.90		NIST Webbook
rinpol	468.88		NIST Webbook
rinpol	468.69		NIST Webbook
rinpol	462.09		NIST Webbook
rinpol	468.44		NIST Webbook
rinpol	469.00		NIST Webbook
rinpol	467.02		NIST Webbook
rinpol	471.16		NIST Webbook
rinpol	468.44		NIST Webbook
rinpol	471.16		NIST Webbook
rinpol	2959.00		NIST Webbook
tb	795.54	K	Joback Method
tc	1051.83	K	Joback Method
tf	442.40 ± 0.80	K	NIST Webbook
tf	452.82	K	Aqueous Solubility Prediction Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.80	J/mol×K	795.54	Joback Method
cpg	614.89	J/mol×K	838.25	Joback Method
cpg	629.30	J/mol×K	880.97	Joback Method
cpg	643.27	J/mol×K	923.68	Joback Method
cpg	657.07	J/mol×K	966.40	Joback Method
cpg	670.94	J/mol×K	1009.11	Joback Method
cpg	685.13	J/mol×K	1051.83	Joback Method
dvisc	0.0028862	Pa×s	581.97	Joback Method

dvisc	0.0031708	Pa×s	539.25	Joback Method
dvisc	0.0026613	Pa×s	624.68	Joback Method
dvisc	0.0024794	Pa×s	667.39	Joback Method
dvisc	0.0023298	Pa×s	710.11	Joback Method
dvisc	0.0022047	Pa×s	752.83	Joback Method
dvisc	0.0020987	Pa×s	795.54	Joback Method
hsubt	127.20 ± 2.40	kJ/mol	413.00	NIST Webbook
hsubt	127.20	kJ/mol	401.00	NIST Webbook
hvapt	93.80	kJ/mol	398.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	553.20	K	11.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	3.66850e+01
Coeff. B	-1.98707e+04
Temperature range (K), min.	545.94
Temperature range (K), max.	633.36

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56495&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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume