

3-Methylcholanthrene

Inchi: InChI=1S/C21H16/c1-13-5-8-17-15(11-13)7-9-18-19-10-6-14-3-2-4-16(21(14)19)12-20(14)1
InchiKey: HVVINGXJHBOTJQ-UHFFFAOYSA-N
Formula: C21H16
SMILES: Cc1ccc2c(ccc3c4c5c(cccc5cc32)CC4)c1
Mol. weight [g/mol]: 268.36

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
log10ws	-7.92		Estimated Solubility Method
logp	5.553		Crippen Method
mcvol	213.750	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
tb	795.54	K	Joback Method
tc	1051.83	K	Joback Method
tf	539.25	K	Joback 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	0.0031708	Pa×s	539.25	Joback Method
dvisc	0.0028862	Pa×s	581.97	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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

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

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