Benz[j]aceanthrylene, 3-methyl-

Other names:	1,2-Dehydro-3-methylcholanthrene
	3-Methylcholanthrylene
	3-Methylbenz(j)aceanthrylene
	Dehydro-3-methylcholanthrene
Inchi:	InChI=1S/C21H14/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:	HUIUEHNRLHPDBT-UHFFFAOYSA-N
Formula:	C21H14
SMILES:	Cc1ccc2cc3c(ccc4ccccc43)c3c2c1C=C3
Mol. weight [g/mol]:	266.34
CAS:	3343-10-0

Physical Properties

Property code	Value	Unit	Source
gf	620.67	kJ/mol	Joback Method
hf	432.70	kJ/mol	Joback Method
hfus	33.68	kJ/mol	Joback Method
hvap	73.19	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	5.938		Crippen Method
mcvol	209.450	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	468.08		NIST Webbook
tb	794.70	K	Joback Method
tc	1053.20	K	Joback Method
tf	540.01	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.91	J/mol×K	794.70	Joback Method
cpg	586.99	J/mol×K	837.78	Joback Method
cpg	600.46	J/mol×K	880.87	Joback Method
cpg	613.57	J/mol×K	923.95	Joback Method

cpg	626.59	J/mol×K	967.03	Joback Method
cpg	639.79	J/mol×K	1010.12	Joback Method
cpg	653.41	J/mol×K	1053.20	Joback Method
dvisc	0.0031877	Pa×s	540.01	Joback Method
dvisc	0.0029417	Pa×s	582.46	Joback Method
dvisc	0.0027446	Pa×s	624.91	Joback Method
dvisc	0.0025833	Pa×s	667.36	Joback Method
dvisc	0.0024492	Pa×s	709.80	Joback Method
dvisc	0.0023360	Pa×s	752.25	Joback Method
dvisc	0.0022394	Pa×s	794.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3343100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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