

Benz[a]anthracene, 9-methyl-

Other names:	6-Methyl-1,2-benzanthracene 9-Methylbenz[a]anthracene
Inchi:	InChI=1S/C19H14/c1-13-6-7-15-12-19-16(11-17(15)10-13)9-8-14-4-2-3-5-18(14)19/h2-13
InchiKey:	KYJPMPXTXCFCRM-UHFFFAOYSA-N
Formula:	C19H14
SMILES:	Cc1ccc2cc3c(ccc4ccccc43)cc2c1
Mol. weight [g/mol]:	242.31
CAS:	2381-16-0

Physical Properties

Property code	Value	Unit	Source
gf	512.57	kJ/mol	Joback Method
hf	339.84	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	67.07	kJ/mol	Joback Method
ie	7.31 ± 0.03	eV	NIST Webbook
ie	7.37	eV	NIST Webbook
log10ws	-7.36		Crippen Method
logp	5.455		Crippen Method
mcvol	196.430	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	416.50		NIST Webbook
rinpol	415.50		NIST Webbook
rinpol	416.50		NIST Webbook
tb	732.68	K	Joback Method
tc	990.82	K	Joback Method
tf	465.97	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.66	J/mol×K	732.68	Joback Method
cpg	533.84	J/mol×K	775.70	Joback Method

cpg	547.92	J/mol×K	818.73	Joback Method
cpg	561.09	J/mol×K	861.75	Joback Method
cpg	573.55	J/mol×K	904.77	Joback Method
cpg	585.49	J/mol×K	947.80	Joback Method
cpg	597.11	J/mol×K	990.82	Joback Method
dvisc	0.0016009	Pa×s	465.97	Joback Method
dvisc	0.0013067	Pa×s	510.42	Joback Method
dvisc	0.0011019	Pa×s	554.87	Joback Method
dvisc	0.0009529	Pa×s	599.33	Joback Method
dvisc	0.0008408	Pa×s	643.78	Joback Method
dvisc	0.0007540	Pa×s	688.23	Joback Method
dvisc	0.0006851	Pa×s	732.68	Joback Method

Sources

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=C2381160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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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