Ethanone, 1-(9-anthracenyl)-

Other names:	9-Acetoanthracene
	9-Acetylanthracene
	Ketone, 9-anthryl methyl
	9-anthryl methyl ketone
Inchi:	InChI=1S/C16H12O/c1-11(17)16-14-8-4-2-6-12(14)10-13-7-3-5-9-15(13)16/h2-10H,1H3
InchiKey:	NXXNVJDXUHMAHU-UHFFFAOYSA-N
Formula:	C16H12O
SMILES:	CC(=O)c1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	220.27
CAS:	784-04-3

Physical Properties

Property code	Value	Unit	Source
ea	1.02 ± 0.10	eV	NIST Webbook
gf	261.37	kJ/mol	Joback Method
hf	109.58	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.196		Crippen Method
mcvol	175.190	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	693.95	K	Joback Method
tc	943.48	K	Joback Method
tf	436.87	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.19	J/mol×K	693.95	Joback Method
cpg	459.14	J/mol×K	735.54	Joback Method
cpg	471.99	J/mol×K	777.13	Joback Method
cpg	483.87	J/mol×K	818.71	Joback Method

cpg	494.92	J/mol×K	860.30	Joback Method
cpg	505.26	J/mol×K	901.89	Joback Method
cpg	515.03	J/mol×K	943.48	Joback Method
dvisc	0.0016094	Pa×s	436.87	Joback Method
dvisc	0.0012091	Pa×s	479.72	Joback Method
dvisc	0.0009519	Pa×s	522.56	Joback Method
dvisc	0.0007771	Pa×s	565.41	Joback Method
dvisc	0.0006528	Pa×s	608.26	Joback Method
dvisc	0.0005611	Pa×s	651.10	Joback Method
dvisc	0.0004914	Pa×s	693.95	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C784043&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
ea: Electron affinity
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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