9-Anthracenecarboxaldehyde

Other names:	9-Anthraldehyde
	9-Anthrylaldehyde
	9-Anthrylcarboxaldehyde
	9-Formylanthracene
	Anthracene-9-carboxaldehyde
	Anthracene-9-aldehyde
	anthracene-9-carbaldehyde
Inchi:	InChI=1S/C15H10O/c16-10-15-13-7-3-1-5-11(13)9-12-6-2-4-8-14(12)15/h1-10H
InchiKey:	YMNKUHIVVMFOFO-UHFFFAOYSA-N
Formula:	C15H10O
SMILES:	O=Cc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	206.24
CAS:	642-31-9

Physical Properties

Property code	Value	Unit	Source
ea	1.02 ± 0.13	eV	NIST Webbook
ea	1.31 ± 0.10	eV	NIST Webbook
gf	282.35	kJ/mol	Joback Method
hf	157.22	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	62.58	kJ/mol	Joback Method
ie	7.67 ± 0.03	eV	NIST Webbook
ie	7.69 ± 0.03	eV	NIST Webbook
ie	7.67	eV	NIST Webbook
log10ws	-5.32		Crippen Method
logp	3.805		Crippen Method
mcvol	161.100	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	356.60		NIST Webbook
rinpol	368.30		NIST Webbook
rinpol	357.30		NIST Webbook
rinpol	2094.00		NIST Webbook
tb	665.86	K	Joback Method
tc	915.62	K	Joback Method
tf	417.67	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.79	J/mol×K	873.99	Joback Method
cpg	442.25	J/mol×K	832.36	Joback Method
cpg	432.02	J/mol×K	790.74	Joback Method
cpg	420.97	J/mol×K	749.11	Joback Method
cpg	408.97	J/mol×K	707.49	Joback Method
cpg	395.89	J/mol×K	665.86	Joback Method
cpg	460.77	J/mol×K	915.62	Joback Method
dvisc	0.0017500	Pa×s	417.67	Joback Method
dvisc	0.0005729	Pa×s	665.86	Joback Method
dvisc	0.0006488	Pa×s	624.50	Joback Method
dvisc	0.0007479	Pa×s	583.13	Joback Method
dvisc	0.0008811	Pa×s	541.76	Joback Method
dvisc	0.0010664	Pa×s	500.40	Joback Method
dvisc	0.0013359	Pa×s	459.04	Joback Method
hfust	17.61	kJ/mol	377.20	NIST Webbook
hsubt	100.60 ± 3.90	kJ/mol	346.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C642319&Units=SI
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

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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