Phenanthrene-9-carboxaldehyde

Other names:	Phenanthrene-9-aldehyde 9-Phenanthrenecarboxaldehyde phenanthrene-9-carbaldehyde
Inchi:	InChI=1S/C15H10O/c16-10-12-9-11-5-1-2-6-13(11)15-8-4-3-7-14(12)15/h1-10H
InchiKey:	QECIGCMPORCORE-UHFFFAOYSA-N
Formula:	C15H10O
SMILES:	O=Cc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]:	206.24
CAS:	4707-71-5

Physical Properties

Property code	Value	Unit	Source
ea	0.72 ± 0.01	eV	NIST Webbook
ea	0.66 ± 0.14	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
log10ws	-5.32		Crippen Method
logp	3.805		Crippen Method
mcvol	161.100	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	354.40		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	354.70		NIST Webbook
rinpol	354.40		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	354.70		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	395.89	J/mol×K	665.86	Joback Method
cpg	408.97	J/mol×K	707.49	Joback Method
cpg	420.97	J/mol×K	749.11	Joback Method
cpg	432.02	J/mol×K	790.74	Joback Method
cpg	442.25	J/mol×K	832.36	Joback Method
cpg	451.79	J/mol×K	873.99	Joback Method
cpg	460.77	J/mol×K	915.62	Joback Method
dvisc	0.0017500	Pa×s	417.67	Joback Method
dvisc	0.0013359	Pa×s	459.04	Joback Method
dvisc	0.0010664	Pa×s	500.40	Joback Method
dvisc	0.0008811	Pa×s	541.76	Joback Method
dvisc	0.0007479	Pa×s	583.13	Joback Method
dvisc	0.0006488	Pa×s	624.50	Joback Method
dvisc	0.0005729	Pa×s	665.86	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=C4707715&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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