1-Pyrenecarboxaldehyde

Other names:	1-Pyrenealdehyde
	1-Pyrenecarbaldehyde
	1-formylpyrene
	3-Formylpyrene
	3-Pyrenealdehyde
	3-Pyrenecarboxaldehyde
	3-Pyrenylaldehyde
	NSC 30811
	pyrene, 1-formyl-
	pyrene-1-carbaldehyde
Inchi:	InChI=1S/C17H10O/c18-10-14-7-6-13-5-4-11-2-1-3-12-8-9-15(14)17(13)16(11)12/h1-10H
InchiKey:	RCYFOPUXRMOLQM-UHFFFAOYSA-N
Formula:	C17H10O
SMILES:	O=Cc1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]:	230.26
CAS:	3029-19-4

Physical Properties

Property code	Value	Unit	Source
gf	390.45	kJ/mol	Joback Method
hf	250.08	kJ/mol	Joback Method
hfus	28.98	kJ/mol	Joback Method
hvap	68.70	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	4.396		Crippen Method
mcvol	174.120	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
rinpol	406.60		NIST Webbook
tb	727.88	K	Joback Method
tc	978.95	K	Joback Method
tf	398.15 ± 2.00	K	NIST Webbook

tf	399.90	K	Experimental and computational thermodynamics of pyrene and 1-pyrenecarboxaldehyde and their photophysical properties
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.33	J/mol×K	727.88	Joback Method
cpg	459.11	J/mol×K	769.73	Joback Method
cpg	470.10	J/mol×K	811.57	Joback Method
cpg	480.48	J/mol×K	853.42	Joback Method
cpg	490.45	J/mol×K	895.26	Joback Method
cpg	500.21	J/mol×K	937.11	Joback Method
cpg	509.95	J/mol×K	978.95	Joback Method
dvisc	0.0028381	Pa×s	491.71	Joback Method
dvisc	0.0025310	Pa×s	531.07	Joback Method
dvisc	0.0022931	Pa×s	570.43	Joback Method
dvisc	0.0021042	Pa×s	609.80	Joback Method
dvisc	0.0019511	Pa×s	649.16	Joback Method
dvisc	0.0018248	Pa×s	688.52	Joback Method
dvisc	0.0017191	Pa×s	727.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3029194&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermodynamics of pyrene and 1-pyrenecarboxaldehyde and their photophysical properties:	https://www.doi.org/10.1016/j.jct.2015.07.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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