1-Acetylpyrene

Other names: Ethanone, 1-(1-pyrenyl)-
Inchi: InChI=1S/C18H12O/c1-11(19)15-9-7-14-6-5-12-3-2-4-13-8-10-16(15)18(14)17(12)13/h2-
InchiKey: KCIJNJVCFPSUBQ-UHFFFAOYSA-N
Formula: C18H12O
SMILES: CC(=O)c1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]: 244.29
CAS: 3264-21-9

Physical Properties

Property code	Value	Unit	Source
gf	369.47	kJ/mol	Joback Method
hf	202.44	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	70.95	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	4.787		Crippen Method
mcvol	188.210	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
tb	755.97	K	Joback Method
tc	1006.60	K	Joback Method
tf	362.65 ± 2.00	K	NIST Webbook
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.07	J/mol×K	755.97	Joback Method
cpg	555.68	J/mol×K	964.83	Joback Method
cpg	544.92	J/mol×K	923.06	Joback Method
cpg	533.97	J/mol×K	881.28	Joback Method
cpg	522.65	J/mol×K	839.51	Joback Method
cpg	510.74	J/mol×K	797.74	Joback Method
cpg	566.44	J/mol×K	1006.60	Joback Method
dvisc	0.0014941	Pa×s	755.97	Joback Method

dvisc	0.0016002	Pa×s	715.13	Joback Method
dvisc	0.0017280	Pa×s	674.28	Joback Method
dvisc	0.0018847	Pa×s	633.44	Joback Method
dvisc	0.0020803	Pa×s	592.60	Joback Method
dvisc	0.0023300	Pa×s	551.75	Joback Method
dvisc	0.0026574	Pa×s	510.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3264219&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume