9-Anthracenecarbonitrile, 10-(acetyloxy)-

Inchi: InChI=1S/C17H11NO2/c1-11(19)20-17-14-8-4-2-6-12(14)16(10-18)13-7-3-5-9-15(13)17/h
InchiKey: BQOUZQNDJTXXIN-UHFFFAOYSA-N
Formula: C17H11NO2
SMILES: CC(=O)Oc1c2ccccc2c(C#N)c2ccccc12
Mol. weight [g/mol]: 261.27
CAS: 47051-16-1

Physical Properties

Property code	Value	Unit	Source
gf	288.34	kJ/mol	Joback Method
hf	110.13	kJ/mol	Joback Method
hfus	30.99	kJ/mol	Joback Method
hvap	80.61	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	3.790		Crippen Method
mcvol	196.530	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
tb	846.31	K	Joback Method
tc	1096.81	K	Joback Method
tf	547.88	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.40	J/mol×K	846.31	Joback Method
cpg	545.34	J/mol×K	888.06	Joback Method
cpg	555.51	J/mol×K	929.81	Joback Method
cpg	565.01	J/mol×K	971.56	Joback Method
cpg	573.96	J/mol×K	1013.31	Joback Method
cpg	582.43	J/mol×K	1055.06	Joback Method
cpg	590.55	J/mol×K	1096.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C47051161&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
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