1-ACETAMIDOPYRENE

Other names: Acetamide, N-1-pyrenyl-
N-Acetyl-1-aminopyrene
N-1-Pyrenylacetamide
Inchi: InChI=1S/C18H13NO/c1-11(20)19-16-10-8-14-6-5-12-3-2-4-13-7-9-15(16)18(14)17(12)13
InchiKey: GJNGMQYHOZFQNX-UHFFFAOYSA-N
Formula: C18H13NO
SMILES: CC(=O)Nc1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]: 259.31

Physical Properties

Property code	Value	Unit	Source
hfus	35.98	kJ/mol	Joback Method
hvap	114.29	kJ/mol	Cheméo Relay (1.0)
ie	7.27	eV	Cheméo Relay (1.0)
log10ws	-4.40		Cheméo Relay (1.0)
logp	4.542		Crippen Method
mcvol	198.190	ml/mol	McGowan Method
tb	727.96	K	Cheméo Relay (1.0)
tf	427.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.33	J/mol×K	806.14	Joback Method
cpg	559.66	J/mol×K	847.35	Joback Method
cpg	571.40	J/mol×K	888.56	Joback Method
cpg	582.72	J/mol×K	929.77	Joback Method
cpg	593.83	J/mol×K	970.98	Joback Method
cpg	604.90	J/mol×K	1012.19	Joback Method
cpg	616.15	J/mol×K	1053.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22755153&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point