3-HYDROXYPYRIDINE MONOACETATE

Other names: 3-Acetoxypyridine
3-Pyridinol, acetate
3-pyridyl acetate
Inchi: InChI=1S/C7H7NO2/c1-6(9)10-7-3-2-4-8-5-7/h2-5H,1H3
InchiKey: QZDWODWEESGPLC-UHFFFAOYSA-N
Formula: C7H7NO2
SMILES: CC(=O)Oc1cccnc1
Mol. weight [g/mol]: 137.14

Physical Properties

Property code	Value	Unit	Source
af	0.4675		Cheméo Relay (1.0)
gf	-118.36	kJ/mol	Cheméo Relay (1.0, beta)
hf	-227.15	kJ/mol	Cheméo Relay (1.0)
hvap	59.20	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-0.53		Cheméo Relay (1.0)
logp	1.007		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4221.06	kPa	Cheméo Relay (1.0, beta)
rinpol	1127.00		NIST Webbook
rinpol	1127.00		NIST Webbook
tb	484.49	K	Cheméo Relay (1.0)
tc	715.66	K	Cheméo Relay (1.0)
tf	289.77	K	Cheméo Relay (1.0)
vc	0.376	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.20	K	1.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C17747432&Units=SI

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume