4-Acetoxy-2-azetidinone

Other names:	2-Azetidinone, 4-(acetyloxy)-
	2-oxoazetidinium 4-acetate
Inchi:	InChI=1S/C5H7NO3/c1-3(7)9-5-2-4(8)6-5/h5H,2H2,1H3,(H,6,8)
InchiKey:	OEYMQQDJCUHKQS-UHFFFAOYSA-N
Formula:	C5H7NO3
SMILES:	CC(=O)OC1CC(O)=N1
Mol. weight [g/mol]:	129.11
CAS:	28562-53-0

Physical Properties

Property code	Value	Unit	Source
gf	-193.76	kJ/mol	Joback Method
hf	-359.64	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	59.81	kJ/mol	Joback Method
log10ws	-0.26		Crippen Method
logp	0.236		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	5228.24	kPa	Joback Method
tb	354.20	K	NIST Webbook
tc	754.88	K	Joback Method
tf	378.33	K	Joback Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.21	J/mol×K	551.12	Joback Method
cpg	230.48	J/mol×K	585.08	Joback Method
cpg	239.28	J/mol×K	619.04	Joback Method
cpg	247.63	J/mol×K	653.00	Joback Method
cpg	255.50	J/mol×K	686.96	Joback Method
cpg	262.90	J/mol×K	720.92	Joback Method
cpg	269.83	J/mol×K	754.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28562530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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