

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

Physical Properties

Property code	Value	Unit	Source
hfus	16.63	kJ/mol	Joback Method
logp	-0.605		Crippen Method
mcpvol	89.440	ml/mol	McGowan Method
tb	354.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.41	J/mol×K	517.47	Joback Method
cpg	210.07	J/mol×K	555.44	Joback Method
cpg	220.33	J/mol×K	593.42	Joback Method
cpg	230.16	J/mol×K	631.39	Joback Method
cpg	239.51	J/mol×K	669.36	Joback Method
cpg	248.37	J/mol×K	707.33	Joback Method
cpg	256.70	J/mol×K	745.31	Joback Method

Sources

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=C28562530&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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