Aspartic acid, N-acetyl-, diethyl ester, L-

Other names: (l) N-acetylaspartic acid, diethyl ester
Inchi: InChI=1S/C10H17NO5/c1-4-15-9(13)6-8(11-7(3)12)10(14)16-5-2/h8H,4-6H2,1-3H3,(H,11
InchiKey: XQGDGRNHLJLQOV-UHFFFAOYSA-N
Formula: C10H17NO5
SMILES: CCOC(=O)CC(N=C(C)O)C(=O)OCC
Mol. weight [g/mol]: 231.25
CAS: 1069-39-2

Physical Properties

Property code	Value	Unit	Source
hf	-824.41	kJ/mol	Joback Method
hvap	75.85	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.848		Crippen Method
mcvol	178.190	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
tb	749.08	K	Joback Method
tc	941.73	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	76.00	kJ/mol	463.00	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1069392&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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