Propanedioic acid, (acetylamino)-, diethyl ester

Other names: (Acetylamino)malonic acid diethyl ester
(Acetylamino)propanedioic acid diethyl ester
2-(Acetylamino)propanedioic acid diethyl ester
Acetamidomalonic acid diethyl ester
Acetaminomalonic acid diethyl ester
Diethyl 2-acetamidomalonate
Diethyl N-acetylaminomalonate
Diethyl a-(acetylamino)malonate
Diethyl acetamidomalonate
Diethyl acetaminomalonate
Diethyl acetylaminomalonate
Diethylester kyseliny acetylaminomalonove
Ethyl acetamidomalonate
Malonic acid, acetamido-, diethyl ester
NSC 7645
Propanedioic acid, 2-(acetylamino)-, 1,3-diethyl ester

Inchi: InChI=1S/C9H15NO5/c1-4-14-8(12)7(10-6(3)11)9(13)15-5-2/h7H,4-5H2,1-3H3,(H,10,11)

InchiKey: ISOLMABRZPQKOV-UHFFFAOYSA-N

Formula: C9H15NO5

SMILES: CCOC(=O)C(NC(C)=O)C(=O)OCC

Mol. weight [g/mol]: 217.22

CAS: 1068-90-2

Physical Properties

Property code	Value	Unit	Source
gf	-484.91	kJ/mol	Joback Method
hf	-783.08	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	66.73	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	-0.383		Crippen Method
mcvol	164.100	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	661.50	K	Joback Method
tc	855.57	K	Joback Method
tf	423.10	K	Joback Method

tt	368.72	K	Heat Capacity and Thermodynamic Property Studies of Diethyl Acetamidomalonate (C9H15NO5)
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.44	J/mol×K	661.50	Joback Method
cpg	446.19	J/mol×K	693.85	Joback Method
cpg	457.31	J/mol×K	726.19	Joback Method
cpg	467.79	J/mol×K	758.54	Joback Method
cpg	477.63	J/mol×K	790.88	Joback Method
cpg	486.80	J/mol×K	823.23	Joback Method
cpg	495.32	J/mol×K	855.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1068902&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Heat Capacity and Thermodynamic Property Studies of Diethyl Acetamidomalonate (C9H15NO5): https://www.doi.org/10.1021/je400159e

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume