

Glycine, N-acetyl-, ethyl ester

Other names:	Acetylglycine ethyl ester Ethyl acetamidoacetate Ethyl N-acetylglycinate N-Acetylglycine ethyl ester Ethyl acetaminoacetate
Inchi:	InChI=1S/C6H11NO3/c1-3-10-6(9)4-7-5(2)8/h3-4H2,1-2H3,(H,7,8)
InchiKey:	AMBDTBHJFINMSE-UHFFFAOYSA-N
Formula:	C6H11NO3
SMILES:	CCOC(=O)CNC(C)=O
Mol. weight [g/mol]:	145.16
CAS:	1906-82-7

Physical Properties

Property code	Value	Unit	Source
gf	-273.81	kJ/mol	Joback Method
hf	-471.08	kJ/mol	Joback Method
hfus	20.78	kJ/mol	Joback Method
hvap	51.29	kJ/mol	Joback Method
log10ws	-0.16		Crippen Method
logp	-0.314		Crippen Method
mcvol	114.390	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	517.01	K	Joback Method
tc	707.99	K	Joback Method
tf	332.13	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.38	J/molxK	517.01	Joback Method
cpg	266.34	J/molxK	548.84	Joback Method
cpg	275.88	J/molxK	580.67	Joback Method
cpg	285.00	J/molxK	612.50	Joback Method

cpg	293.70	J/mol×K	644.33	Joback Method
cpg	301.98	J/mol×K	676.16	Joback Method
cpg	309.84	J/mol×K	707.99	Joback Method
hvapt	69.40	kJ/mol	424.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	533.20	K	94.90	NIST Webbook

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=C1906827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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