

Ethyl acetamidocyanoacetate

Other names:	Ethyl acetaminocyanoacetate Acetic acid, (acetylamino)cyano-, ethyl ester Ethyl 2-acetamido-2-cyanoacetate Glycine, N-acetyl-2-cyano-, ethyl ester
Inchi:	InChI=1S/C7H10N2O3/c1-3-12-7(11)6(4-8)9-5(2)10/h6H,3H2,1-2H3,(H,9,10)
InchiKey:	SLIRLABNGAZSHX-UHFFFAOYSA-N
Formula:	C7H10N2O3
SMILES:	CCOC(=O)C(C#N)NC(C)=O
Mol. weight [g/mol]:	170.17
CAS:	4977-62-2

Physical Properties

Property code	Value	Unit	Source
gf	-134.65	kJ/mol	Joback Method
hf	-332.12	kJ/mol	Joback Method
hfus	21.35	kJ/mol	Joback Method
hvap	63.60	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	-0.422		Crippen Method
mcvol	129.860	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	641.53	K	Joback Method
tc	848.87	K	Joback Method
tf	393.39	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.66	J/molxK	641.53	Joback Method
cpg	329.93	J/molxK	676.09	Joback Method
cpg	338.66	J/molxK	710.64	Joback Method
cpg	346.85	J/molxK	745.20	Joback Method
cpg	354.52	J/molxK	779.76	Joback Method

cpg	361.65	J/mol×K	814.31	Joback Method
cpg	368.25	J/mol×K	848.87	Joback Method

Sources

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=C4977622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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