

2-Propenoic acid, 2-cyano-3-ethoxy-, ethyl ester

Other names:	Acrylic acid, 2-cyano-3-ethoxy-, ethyl ester Ethyl «alpha»-(ethoxymethylene)-«alpha»-cyanoacetate Ethyl (ethoxymethylene)cyanoacetate Ethyl cyano(ethoxymethylene)acetate Ethyl 2-cyano-3-ethoxyacrylate Ethyl 3-ethoxy-2-cyanoacrylate 2-(Ethoxymethylene)-2-cyanoacetic acid ethyl ester Ethyl 2-cyano-3-ethoxy-2-propenoate NSC 27797
Inchi:	InChI=1S/C8H11NO3/c1-3-11-6-7(5-9)8(10)12-4-2/h6H,3-4H2,1-2H3/b7-6+
InchiKey:	KTMGNAIGXYODKQ-VOTSOKGWSA-N
Formula:	C8H11NO3
SMILES:	CCOC=C(C#N)C(=O)OCC
Mol. weight [g/mol]:	169.18
CAS:	94-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-117.59	kJ/mol	Joback Method
hf	-313.16	kJ/mol	Joback Method
hfus	20.85	kJ/mol	Joback Method
hvap	55.48	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.993		Crippen Method
mcvol	133.970	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	587.27	K	Joback Method
tc	789.84	K	Joback Method
tf	320.26	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	312.20	J/mol×K	587.27	Joback Method
cpg	322.34	J/mol×K	621.03	Joback Method
cpg	332.00	J/mol×K	654.79	Joback Method
cpg	341.19	J/mol×K	688.56	Joback Method
cpg	349.89	J/mol×K	722.32	Joback Method
cpg	358.13	J/mol×K	756.08	Joback Method
cpg	365.89	J/mol×K	789.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.70	K	4.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

vc: Critical Volume

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