

Carbamic acid, (cyanoacetyl)-, ethyl ester

Other names:	Cyanoacetylurethan Ethyl cyanacetylcarbamate Ethyl cyanoacetylcarbamate N-Cyanoacetylurethane 2-Cyanoacetylurethane N-Cyanoacetyl ethyl carbamate 2-Cyanoacetylcarbamic acid, ethyl ester
Inchi:	InChI=1S/C6H8N2O3/c1-2-11-6(10)8-5(9)3-4-7/h2-3H2,1H3,(H,8,9,10)
InchiKey:	HSOGVWWWGVFXGF-UHFFFAOYSA-N
Formula:	C6H8N2O3
SMILES:	CCOC(=O)NC(=O)CC#N
Mol. weight [g/mol]:	156.14
CAS:	6629-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-140.63	kJ/mol	Joback Method
hf	-306.20	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	61.77	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.173		Crippen Method
mcvol	115.770	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	619.09	K	Joback Method
tc	825.58	K	Joback Method
tf	397.12	K	Joback Method
vc	0.463	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.84	J/mol×K	619.09	Joback Method
cpg	281.99	J/mol×K	653.51	Joback Method

cpg	289.69	J/mol×K	687.92	Joback Method
cpg	296.94	J/mol×K	722.34	Joback Method
cpg	303.74	J/mol×K	756.75	Joback Method
cpg	310.09	J/mol×K	791.17	Joback Method
cpg	315.98	J/mol×K	825.58	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=C6629045&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/67-266-3/Carbamic-acid-cyanoacetyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-27 07:45:23.217964559 +0000 UTC m=+16493172.138541923.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.