2-Propenoic acid, 2-cyano-, methyl ester

Other names:	2-Propenoic acid, 2-cyano-, methyl ester
	Acrylic acid, 2-cyano-, methyl ester
	«alpha»-Cyanoacrylic acid, methyl ester
	Adhere
	Coapt.
	Cyanolit
	Eastman 910
	Eastman 910 Adhesive
	Eastman 910 monomer
	Mecrilat
	Methyl «alpha»-cyanoacrylate
	Methyl cyanoacrylate
	Methyl 2-cyanoacrylate
	2-Cyanoacrylic acid, methyl ester
	Coapt
	Mecrilate
	Methyl ester of 2-cyano-2-propenoic acid
Inchi:	InChI=1S/C5H5NO2/c1-4(3-6)5(7)8-2/h1H2,2H3
InchiKey:	MWCLLHOVUTZFKS-UHFFFAOYSA-N
Formula:	C5H5NO2
SMILES:	C=C(C#N)C(=O)OC
Mol. weight [g/mol]:	111.10

Physical Properties

Property code	Value	Unit	Source
af	0.4522		Cheméo Relay (1.0)
hf	-109.24	kJ/mol	Cheméo Relay (1.0)
hfus	10.41	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Cheméo Relay (1.0)
ie	10.98 ± 0.05	eV	NIST Webbook
log10ws	-0.49		Cheméo Relay (1.0)
logp	0.239		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	431.33	K	Cheméo Relay (1.0)
tc	620.41	K	Cheméo Relay (1.0)
tf	355.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.05	J/mol×K	488.73	Joback Method
cpg	172.53	J/mol×K	523.55	Joback Method
cpg	178.73	J/mol×K	558.37	Joback Method
cpg	184.65	J/mol×K	593.20	Joback Method
cpg	190.28	J/mol×K	628.02	Joback Method
cpg	195.63	J/mol×K	662.84	Joback Method
cpg	200.69	J/mol×K	697.66	Joback Method
hvapt	57.80	kJ/mol	270.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	320.70	K	0.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C137053&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity

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
ie:	Ionization energy
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