Ethyl 2-cyanoacrylate

Inchi: InChI=1S/C6H7NO2/c1-3-9-6(8)5(2)4-7/h2-3H2,1H3
InchiKey: FGBJXOREULPLGL-UHFFFAOYSA-N
Formula: C6H7NO2
SMILES: C=C(C#N)C(=O)OCC
Mol. weight [g/mol]: 125.13
CAS: 7085-85-0

Physical Properties

Property code	Value	Unit	Source
hf	-160.73	kJ/mol	Cheméo Relay (1.0)
hfus	14.58	kJ/mol	Joback Method
hvap	52.02	kJ/mol	Cheméo Relay (1.0)
ie	10.46	eV	Cheméo Relay (1.0)
logp	0.629		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	444.67	K	Cheméo Relay (1.0)
tc	637.26	K	Cheméo Relay (1.0)
tf	250.90	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	3.71610e+01
Coeff. B	4.33720e-01
Coeff. C	-2.02200e-04
Coeff. D	1.60000e-08
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
ie:	Ionization energy
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

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