Ethyl 2-cyanoacetoacetate

Other names:	Ethyl a-cyanoacetoacetate
	Ethyl «alpha»-cyanoacetoacetate
Inchi:	InChI=1S/C7H9NO3/c1-3-11-7(10)6(4-8)5(2)9/h6H,3H2,1-2H3
InchiKey:	NWOKVFOTWMZMHL-UHFFFAOYSA-N
Formula:	C7H9NO3
SMILES:	CCOC(=O)C(C#N)C(C)=O
Mol. weight [g/mol]:	155.15
CAS:	634-55-9

Physical Properties

Property code	Value	Unit	Source
chs	-3504.00	kJ/mol	NIST Webbook
gf	-224.04	kJ/mol	Joback Method
hf	-385.59	kJ/mol	Joback Method
hfs	-536.80	kJ/mol	NIST Webbook
hfus	16.25	kJ/mol	Joback Method
hvap	57.17	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	0.278		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	591.36	K	Joback Method
tc	798.81	K	Joback Method
tf	340.73	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.23	J/mol×K	591.36	Joback Method
cpg	286.29	J/mol×K	625.94	Joback Method
cpg	294.87	J/mol×K	660.51	Joback Method
cpg	302.99	J/mol×K	695.09	Joback Method
cpg	310.64	J/mol×K	729.66	Joback Method

cpg	317.82	J/mol×K	764.24	Joback Method
cpg	324.52	J/mol×K	798.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.00 ± 1.00	K	2.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C634559&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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