(E)-Methyl 3-cyano-2-propenoate

Inchi: InChI=1S/C5H5NO2/c1-8-5(7)3-2-4-6/h2-3H,1H3/b3-2+
InchiKey: AJXIQWIGXITQSV-NSCUHMNNSA-N
Formula: C5H5NO2
SMILES: COC(=O)C=CC#N
Mol. weight [g/mol]: 111.10
CAS: 925-56-4

Physical Properties

Property code	Value	Unit	Source
gf	-29.30	kJ/mol	Joback Method
hf	-109.23	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Joback Method
hvap	46.32	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.239		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	496.33	K	Joback Method
tc	706.59	K	Joback Method
tf	278.18	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.90	J/mol×K	496.33	Joback Method
cpg	171.44	J/mol×K	531.37	Joback Method
cpg	177.66	J/mol×K	566.42	Joback Method
cpg	183.57	J/mol×K	601.46	Joback Method
cpg	189.16	J/mol×K	636.51	Joback Method
cpg	194.46	J/mol×K	671.55	Joback Method
cpg	199.46	J/mol×K	706.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C925564&Units=SI
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

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