2-Propenoic acid, 2-cyano-3-phenyl-, methyl ester

Other names: Cinnamic acid, «alpha»-cyano-, methyl ester
Methyl «alpha»-cyanocinnamate
Benzal-cyanessigsaeure-methyl-ester
«alpha»-Cyanocinnamic acid methyl ester
F 2378
Methyl benzalcyanoacetate
2-Cyano-3-phenyl-propensaeuremethylester
2-Cyano-3-phenyl-2-propenoic acid, methyl ester
Methyl 2-cyano-3-phenyl-2-propenoate
NSC 163367

Inchi: InChI=1S/C11H9NO2/c1-14-11(13)10(8-12)7-9-5-3-2-4-6-9/h2-7H,1H3/b10-7+

InchiKey: XLNFLJOWTRDNCX-JXMROGBWSA-N

Formula: C11H9NO2

SMILES: COC(=O)C(C#N)=Cc1ccccc1

Mol. weight [g/mol]: 187.19

CAS: 3695-84-9

Physical Properties

Property code	Value	Unit	Source
gf	125.08	kJ/mol	Joback Method
hf	-6.33	kJ/mol	Joback Method
hfus	21.47	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.767		Crippen Method
mcvol	146.610	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	660.17	K	Joback Method
tc	896.86	K	Joback Method
tf	358.26	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.41	J/mol×K	660.17	Joback Method
cpg	360.59	J/mol×K	699.62	Joback Method
cpg	370.93	J/mol×K	739.07	Joback Method
cpg	380.48	J/mol×K	778.51	Joback Method
cpg	389.27	J/mol×K	817.96	Joback Method
cpg	397.36	J/mol×K	857.41	Joback Method
cpg	404.80	J/mol×K	896.86	Joback Method

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=C3695849&Units=SI

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