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

Other names: Ethyl «alpha»-cyanocinnamate
Ethyl-«alpha»-benzalcyanoacetate
«alpha»-Cyanocinnamic acid ethyl ester
Cinnamic acid, «alpha»-cyano-, ethyl ester
Ethyl benzylidenecyanoacetate
Cinnamic acid, alpha-cyano-, ethyl ester
Benzylidenecyanoacetic acid ethyl ester
Ethyl alpha-benzylidenecyanoacetate
Ethyl alpha-cyanocinnamate
Ethyl 2-benzylidene-2-cyanoacetate
Ethyl 2-cyanocinnamate
Ethyl 3-phenyl-2-cyano-2-propenoate
2-Cyano-3-phenyl- 2-propenoic acid, ethyl ester
Ethyl 2-cyano-3-phenyl-2-propenoate
NSC 8904

Inchi: InChI=1S/C12H11NO2/c1-2-15-12(14)11(9-13)8-10-6-4-3-5-7-10/h3-8H,2H2,1H3/b11-8+

InchiKey: KCDAMWRCUXGACP-DHZHZOJOSA-N

Formula: C12H11NO2

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

Mol. weight [g/mol]: 201.22

CAS: 2025-40-3

Physical Properties

Property code	Value	Unit	Source
gf	133.50	kJ/mol	Joback Method
hf	-26.97	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.157		Crippen Method
mcvol	160.700	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
tb	683.05	K	Joback Method
tc	915.03	K	Joback Method
tf	369.53	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.39	J/mol×K	683.05	Joback Method
cpg	410.28	J/mol×K	721.71	Joback Method
cpg	421.29	J/mol×K	760.38	Joback Method
cpg	431.48	J/mol×K	799.04	Joback Method
cpg	440.90	J/mol×K	837.71	Joback Method
cpg	449.59	J/mol×K	876.37	Joback Method
cpg	457.60	J/mol×K	915.03	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2025403&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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