

Ethyl 2-cyano-3-phenyl delta²-pentenoate

Other names:	Ethyl 2-cyano-3-phenyl delta
Inchi:	InChI=1S/C14H15NO2/c1-3-12(11-8-6-5-7-9-11)13(10-15)14(16)17-4-2/h5-9H,3-4H2,1-2
InchiKey:	LYBDDDYNWSIADW-SEYXRHQNSA-N
Formula:	C14H15NO2
SMILES:	CCOC(=O)C(C#N)=C(CC)c1ccccc1
Mol. weight [g/mol]:	229.27
CAS:	14442-48-9

Physical Properties

Property code	Value	Unit	Source
gf	141.79	kJ/mol	Joback Method
hf	-78.04	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	68.79	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.937		Crippen Method
mcvol	188.880	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
tb	728.69	K	Joback Method
tc	955.87	K	Joback Method
tf	378.11	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.12	J/molxK	728.69	Joback Method
cpg	513.30	J/molxK	766.55	Joback Method
cpg	525.54	J/molxK	804.42	Joback Method
cpg	536.90	J/molxK	842.28	Joback Method
cpg	547.44	J/molxK	880.14	Joback Method
cpg	557.21	J/molxK	918.01	Joback Method
cpg	566.25	J/molxK	955.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14442489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvpap:	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

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