

Benzeneacetic acid, «alpha»-cyano-, ethyl ester

Other names:	Acetic acid, cyanophenyl-, ethyl ester Ethyl cyanophenylacetate Phenylcyanoacetic acid ethyl ester Ethyl phenylcyanoacetate Ethyl «alpha»-cyanophenylacetate Ethyl 2-cyano-2-phenylacetate Ethyl «alpha»-cyano-«alpha»-phenylacetate Ethyl ester of «alpha»-cyanobenzeneacetic acid
Inchi:	InChI=1S/C11H11NO2/c1-2-14-11(13)10(8-12)9-6-4-3-5-7-9/h3-7,10H,2H2,1H3
InchiKey:	SXIRJEDGTAKGKU-UHFFFAOYSA-N
Formula:	C11H11NO2
SMILES:	CCOC(=O)C(C#N)c1ccccc1
Mol. weight [g/mol]:	189.21
CAS:	4553-07-5

Physical Properties

Property code	Value	Unit	Source
gf	50.97	kJ/mol	Joback Method
hf	-119.04	kJ/mol	Joback Method
hfus	19.06	kJ/mol	Joback Method
hvap	61.60	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.857		Crippen Method
mcvol	150.910	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	548.20	K	NIST Webbook
tc	883.61	K	Joback Method
tf	362.30	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.73	J/molxK	655.69	Joback Method

cpg	384.74	J/mol×K	693.68	Joback Method
cpg	395.92	J/mol×K	731.66	Joback Method
cpg	406.26	J/mol×K	769.65	Joback Method
cpg	415.82	J/mol×K	807.64	Joback Method
cpg	424.60	J/mol×K	845.62	Joback Method
cpg	432.63	J/mol×K	883.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4553075&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

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