3-(3-Nitrophenyl)propenoic acid, ethyl ester

Other names:	Ethyl-3-nitrocinnamate
	Ethyl-m-nitrocinnamate
	2-Propenoic acid, 3-(3-nitrophenyl)-, ethyl ester
	Cinnamic acid, m-nitro-, ethyl ester
	m-Nitro-cinnamic acid, ethyl ester
	Ethyl 3-(3-nitrophenyl)-2-propenoate
Inchi:	InChI=1S/C11H11NO4/c1-2-16-11(13)7-6-9-4-3-5-10(8-9)12(14)15/h3-8H,2H2,1H3/b7-6-
InchiKey:	QZEPRSLOWNHADS-VOTSOKGWSA-N
Formula:	C11H11NO4
SMILES:	CCOC(=O)C=Cc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	221.21
CAS:	5396-71-4

Physical Properties

Property code	Value	Unit	Source
gf	26.37	kJ/mol	Joback Method
hf	-183.65	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	68.72	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.171		Crippen Method
mcvol	162.650	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
tb	715.03	K	Joback Method
tc	956.93	K	Joback Method
tf	463.36	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.70	J/mol×K	715.03	Joback Method
cpg	433.77	J/mol×K	755.35	Joback Method
cpg	444.88	J/mol×K	795.66	Joback Method

cpg	455.10	J/mol×K	835.98	Joback Method
cpg	464.47	J/mol×K	876.29	Joback Method
cpg	473.04	J/mol×K	916.61	Joback Method
cpg	480.85	J/mol×K	956.93	Joback Method

Sources

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=C5396714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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