Hydrocinnamic acid, «beta»-methyl-p-nitro-, methyl ester

Other names: Methyl 3-(4-nitrophenyl)butanoate
3-(4-Nitrophenyl)butanoic acid methyl ester
Inchi: InChI=1S/C11H13NO4/c1-8(7-11(13)16-2)9-3-5-10(6-4-9)12(14)15/h3-6,8H,7H2,1-2H3
InchiKey: LGXBWSXGLXOQDJ-UHFFFAOYSA-N
Formula: C11H13NO4
SMILES: COC(=O)CC(C)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 223.23
CAS: 24254-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-56.29	kJ/mol	Joback Method
hf	-306.15	kJ/mol	Joback Method
hfus	28.52	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.261		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
tb	710.43	K	Joback Method
tc	947.65	K	Joback Method
tf	453.44	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.27	J/mol×K	710.43	Joback Method
cpg	459.28	J/mol×K	749.97	Joback Method
cpg	471.29	J/mol×K	789.50	Joback Method
cpg	482.33	J/mol×K	829.04	Joback Method
cpg	492.43	J/mol×K	868.58	Joback Method
cpg	501.61	J/mol×K	908.12	Joback Method
cpg	509.90	J/mol×K	947.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24254613&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

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