4-Nitrophenyl-«beta»-phenylpropionate

Other names: 3-Phenylpropionic acid, 4-nitrophenyl ester
Inchi: InChI=1S/C15H13NO4/c17-15(11-6-12-4-2-1-3-5-12)20-14-9-7-13(8-10-14)16(18)19/h1-5
InchiKey: GYFYEPQCKDJYCF-UHFFFAOYSA-N
Formula: C15H13NO4
SMILES: O=C(CCc1ccccc1)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 271.27
CAS: 17895-71-5

Physical Properties

Property code	Value	Unit	Source
gf	92.24	kJ/mol	Joback Method
hf	-146.90	kJ/mol	Joback Method
hfus	36.45	kJ/mol	Joback Method
hvap	79.95	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.133		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	2253.00		NIST Webbook
rinpol	2253.00		NIST Webbook
tb	829.07	K	Joback Method
tc	1084.98	K	Joback Method
tf	539.94	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.32	J/mol×K	829.07	Joback Method
cpg	576.75	J/mol×K	871.72	Joback Method
cpg	587.93	J/mol×K	914.37	Joback Method
cpg	597.92	J/mol×K	957.02	Joback Method
cpg	606.79	J/mol×K	999.67	Joback Method
cpg	614.61	J/mol×K	1042.33	Joback Method

cpg	621.45	J/mol×K	1084.98	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=C17895715&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume