Phenyl-4-nitrophenylacetic acid, methyl ester

Inchi: InChI=1S/C15H13NO4/c1-20-15(17)14(11-5-3-2-4-6-11)12-7-9-13(10-8-12)16(18)19/h2-1
InchiKey: JMRXEYLTVZUDJR-UHFFFAOYSA-N
Formula: C15H13NO4
SMILES: COC(=O)C(c1ccccc1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 271.27

Physical Properties

Property code	Value	Unit	Source
gf	89.80	kJ/mol	Joback Method
hf	-152.18	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.900		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2205.00		NIST Webbook
tb	828.63	K	Joback Method
tc	1089.25	K	Joback Method
tf	524.94	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.92	J/mol×K	828.63	Joback Method
cpg	577.56	J/mol×K	872.07	Joback Method
cpg	588.88	J/mol×K	915.50	Joback Method
cpg	598.95	J/mol×K	958.94	Joback Method
cpg	607.85	J/mol×K	1002.38	Joback Method
cpg	615.64	J/mol×K	1045.82	Joback Method
cpg	622.41	J/mol×K	1089.25	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=R190139&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

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