o-Toluic acid, 4-nitrophenyl ester

Other names: o-Toluylic acid, 4-nitrophenyl ester
Inchi: InChI=1S/C14H11NO4/c1-10-4-2-3-5-13(10)14(16)19-12-8-6-11(7-9-12)15(17)18/h2-9H,
InchiKey: GCPPQGAWBTYPFF-UHFFFAOYSA-N
Formula: C14H11NO4
SMILES: Cc1ccccc1C(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 257.24

Physical Properties

Property code	Value	Unit	Source
gf	74.19	kJ/mol	Joback Method
hf	-137.73	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	78.38	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.122		Crippen Method
mcvol	185.460	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	811.17	K	Joback Method
tc	1073.33	K	Joback Method
tf	541.19	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.87	J/mol×K	811.17	Joback Method
cpg	520.90	J/mol×K	854.86	Joback Method
cpg	531.68	J/mol×K	898.56	Joback Method
cpg	541.27	J/mol×K	942.25	Joback Method
cpg	549.73	J/mol×K	985.95	Joback Method
cpg	557.11	J/mol×K	1029.64	Joback Method
cpg	563.48	J/mol×K	1073.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307460&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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