4-Nitrobenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C15H13NO4/c1-10-7-11(2)9-14(8-10)20-15(17)12-3-5-13(6-4-12)16(18)19/h3-9
InchiKey: HSVPQSQPHHVITQ-UHFFFAOYSA-N
Formula: C15H13NO4
SMILES: Cc1cc(C)cc(OC(=O)c2ccc([N+](=O)[O-])cc2)c1
Mol. weight [g/mol]: 271.27

Physical Properties

Property code	Value	Unit	Source
gf	72.98	kJ/mol	Joback Method
hf	-169.84	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	81.27	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.431		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	839.03	K	Joback Method
tc	1096.31	K	Joback Method
tf	564.98	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.10	J/mol×K	839.03	Joback Method
cpg	573.34	J/mol×K	881.91	Joback Method
cpg	584.34	J/mol×K	924.79	Joback Method
cpg	594.14	J/mol×K	967.67	Joback Method
cpg	602.79	J/mol×K	1010.55	Joback Method
cpg	610.34	J/mol×K	1053.43	Joback Method
cpg	616.83	J/mol×K	1096.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308011&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume