4-Nitrobenzoic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C14H11NO5/c1-19-12-6-8-13(9-7-12)20-14(16)10-2-4-11(5-3-10)15(17)18/h2-9
InchiKey: RUPXYSFECLCNRL-UHFFFAOYSA-N
Formula: C14H11NO5
SMILES: COc1ccc(OC(=O)c2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 273.24

Physical Properties

Property code	Value	Unit	Source
gf	-30.81	kJ/mol	Joback Method
hf	-269.95	kJ/mol	Joback Method
hfus	34.66	kJ/mol	Joback Method
hvap	80.79	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	2.823		Crippen Method
mcvol	191.330	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
tb	833.59	K	Joback Method
tc	1091.42	K	Joback Method
tf	563.42	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.41	J/mol×K	833.59	Joback Method
cpg	544.88	J/mol×K	876.56	Joback Method
cpg	555.06	J/mol×K	919.53	Joback Method
cpg	563.97	J/mol×K	962.50	Joback Method
cpg	571.63	J/mol×K	1005.48	Joback Method
cpg	578.07	J/mol×K	1048.45	Joback Method
cpg	583.33	J/mol×K	1091.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308012&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

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