bis-(2-Nitrophenyl)acetic acid, methyl ester

Inchi: InChI=1S/C15H12N2O6/c1-23-15(18)14(10-6-2-4-8-12(10)16(19)20)11-7-3-5-9-13(11)17
InchiKey: RRPCEONSNZSQIH-UHFFFAOYSA-N
Formula: C15H12N2O6
SMILES: COC(=O)C(c1ccccc1[N+](=O)[O-])c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 316.27

Physical Properties

Property code	Value	Unit	Source
gf	115.72	kJ/mol	Joback Method
hf	-174.41	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	96.81	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	2.808		Crippen Method
mcvol	216.970	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		NIST Webbook
tb	985.45	K	Joback Method
tc	1260.43	K	Joback Method
tf	681.07	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.67	J/mol×K	985.45	Joback Method
cpg	656.37	J/mol×K	1031.28	Joback Method
cpg	663.79	J/mol×K	1077.11	Joback Method
cpg	670.00	J/mol×K	1122.94	Joback Method
cpg	675.09	J/mol×K	1168.77	Joback Method
cpg	679.15	J/mol×K	1214.60	Joback Method
cpg	682.25	J/mol×K	1260.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190020&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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