

2-Nitrophenyl-3-nitrophenylacetic acid, methyl ester

Inchi:	InChI=1S/C15H12N2O6/c1-23-15(18)14(10-5-4-6-11(9-10)16(19)20)12-7-2-3-8-13(12)17
InchiKey:	OZFHTDWITPKMJT-UHFFFAOYSA-N
Formula:	C15H12N2O6
SMILES:	COC(=O)C(c1cccc([N+](=O)[O-])c1)c1cccc1[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
mvol	216.970	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2466.00		NIST Webbook
rinpol	2466.00		NIST Webbook
tb	985.45	K	Joback Method
tc	1260.43	K	Joback Method
tf	681.07	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R189961&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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