ortho-«alpha»-Hydroxymononitrodiphenylacetic acid, methyl ester

Other names: Phenyl-2-nitrophenyl-hydroxyacetic acid, methyl ester
Inchi: InChI=1S/C15H13NO5/c1-21-14(17)15(18,11-7-3-2-4-8-11)12-9-5-6-10-13(12)16(19)20/h
InchiKey: JPDKSFMTVLDBEK-UHFFFAOYSA-N
Formula: C15H13NO5
SMILES: COC(=O)C(O)(c1ccccc1)c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 287.27

Physical Properties

Property code	Value	Unit	Source
gf	-41.74	kJ/mol	Joback Method
hf	-307.88	kJ/mol	Joback Method
hfus	33.12	kJ/mol	Joback Method
hvap	95.33	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.004		Crippen Method
mcvol	205.420	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2183.00		NIST Webbook
tb	918.02	K	Joback Method
tc	1166.36	K	Joback Method
tf	603.18	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.17	J/mol×K	918.02	Joback Method
cpg	618.63	J/mol×K	959.41	Joback Method
cpg	627.15	J/mol×K	1000.80	Joback Method
cpg	634.83	J/mol×K	1042.19	Joback Method
cpg	641.77	J/mol×K	1083.58	Joback Method

cpg	648.07	J/mol×K	1124.97	Joback Method
cpg	653.83	J/mol×K	1166.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190104&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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