1,3-Benzenedicarboxylic acid, 5-nitro-, bis(1-methylethyl) ester

Other names: Nitrothal-isopropyl
Nitrothol isopropyl
BAS 30000F
Bis(1-methylethyl) 5-nitro-1,3-benzenedicarboxylate
Nitrothale-isopropyl
diisopropyl 5-nitroisophthalate

Inchi: InChI=1S/C14H17NO6/c1-8(2)20-13(16)10-5-11(14(17)21-9(3)4)7-12(6-10)15(18)19/h5-9

InchiKey: VJAWBEFMCIINFU-UHFFFAOYSA-N

Formula: C14H17NO6

SMILES: CC(C)OC(=O)c1cc(C(=O)OC(C)C)cc([N+](=O)[O-])c1

Mol. weight [g/mol]: 295.29

CAS: 10552-74-6

Physical Properties

Property code	Value	Unit	Source
gf	-277.02	kJ/mol	Joback Method
hf	-629.62	kJ/mol	Joback Method
hfus	35.17	kJ/mol	Joback Method
hvap	84.48	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	2.725		Crippen Method
mcvol	216.660	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	2009.00		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	2009.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	859.90	K	Joback Method
tc	1092.56	K	Joback Method
tf	556.93	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.02	J/mol×K	859.90	Joback Method
cpg	653.92	J/mol×K	898.68	Joback Method
cpg	664.61	J/mol×K	937.45	Joback Method
cpg	674.11	J/mol×K	976.23	Joback Method
cpg	682.41	J/mol×K	1015.01	Joback Method
cpg	689.54	J/mol×K	1053.78	Joback Method
cpg	695.49	J/mol×K	1092.56	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10552746&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

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