1,3-Benzenedicarboxylic acid, 5-nitro-, dimethyl ester

Other names: Dimethyl 5-nitroisophthalate
Isophthalic acid, 5-nitro-, dimethyl ester
5-Nitroisophthalic acid, dimethyl ester

Inchi: InChI=1S/C10H9NO6/c1-16-9(12)6-3-7(10(13)17-2)5-8(4-6)11(14)15/h3-5H,1-2H3

InchiKey: GGTSJKFPGKFLCZ-UHFFFAOYSA-N

Formula: C10H9NO6

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

Mol. weight [g/mol]: 239.18

CAS: 13290-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-305.82	kJ/mol	Joback Method
hf	-536.50	kJ/mol	Joback Method
hfus	31.85	kJ/mol	Joback Method
hvap	76.36	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.168		Crippen Method
mcvol	160.300	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	769.26	K	Joback Method
tc	1009.15	K	Joback Method
tf	541.85	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.39	J/mol×K	769.26	Joback Method
cpg	436.56	J/mol×K	809.24	Joback Method
cpg	445.78	J/mol×K	849.22	Joback Method
cpg	454.05	J/mol×K	889.21	Joback Method
cpg	461.36	J/mol×K	929.19	Joback Method
cpg	467.69	J/mol×K	969.17	Joback Method

cpg	473.04	J/mol×K	1009.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13290965&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume