

Benzoic acid, 4-nitro-, 1-methylethyl ester

Other names:	4-Nitrobenzoic acid, isopropyl ester Isopropyl 4-nitrobenzoate Benzoic acid, 4-nitro, isopropyl ester
Inchi:	InChI=1S/C10H11NO4/c1-7(2)15-10(12)8-3-5-9(6-4-8)11(13)14/h3-7H,1-2H3
InchiKey:	JSZSPHFHMMXJEU-UHFFFAOYSA-N
Formula:	C10H11NO4
SMILES:	CC(C)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	209.20
CAS:	13756-40-6

Physical Properties

Property code	Value	Unit	Source
gf	-64.71	kJ/mol	Joback Method
hf	-285.51	kJ/mol	Joback Method
hfus	25.93	kJ/mol	Joback Method
hvap	66.15	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.160		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
ripol	1536.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2339.00		NIST Webbook
ripol	2256.00		NIST Webbook
ripol	2256.00		NIST Webbook
ripol	2287.00		NIST Webbook
tb	687.55	K	Joback Method
tc	929.72	K	Joback Method
tf	442.17	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.71	J/molxK	687.55	Joback Method
cpg	408.14	J/molxK	727.91	Joback Method
cpg	419.60	J/molxK	768.27	Joback Method
cpg	430.12	J/molxK	808.64	Joback Method
cpg	439.73	J/molxK	849.00	Joback Method
cpg	448.44	J/molxK	889.36	Joback Method
cpg	456.29	J/molxK	929.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13756406&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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