4-Nitrobenzoic acid, 2-methylpropyl ester

Other names:	Benzoic acid, p-nitro-, isobutyl ester
	Benzoic acid, 4-nitro-, 2-methylpropyl ester
	Isobutyl p-nitrobenzoate
	4-Nitrobenzoic acid, 2-methylpropyl ester
Inchi:	InChI=1S/C11H13NO4/c1-8(2)7-16-11(13)9-3-5-10(6-4-9)12(14)15/h3-6,8H,7H2,1-2H3
InchiKey:	DCZWILGYHRWANR-UHFFFAOYSA-N
Formula:	C11H13NO4
SMILES:	CC(C)COC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	223.23

Physical Properties

Property code	Value	Unit	Source
hf	-357.62	kJ/mol	Cheméo Relay (1.0)
hfus	28.52	kJ/mol	Joback Method
hvap	85.43	kJ/mol	Cheméo Relay (1.0)
ie	9.89	eV	Cheméo Relay (1.0)
log10ws	-3.84		Cheméo Relay (1.0)
logp	2.408		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
rinpol	1657.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1653.00		NIST Webbook
ripol	2409.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2454.00		NIST Webbook
ripol	2395.00		NIST Webbook
ripol	2395.00		NIST Webbook
tb	573.75	K	Cheméo Relay (1.0)
tf	330.79	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	446.27	J/mol×K	710.43	Joback Method
cpg	459.28	J/mol×K	749.97	Joback Method
cpg	471.29	J/mol×K	789.50	Joback Method
cpg	482.33	J/mol×K	829.04	Joback Method
cpg	492.43	J/mol×K	868.58	Joback Method
cpg	501.61	J/mol×K	908.12	Joback Method
cpg	509.90	J/mol×K	947.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99785&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point