4-Nitrobenzoic acid, 2-butyl ester

Other names:	Benzoic acid, 4-nitro, 1-methylpropyl ester
	Benzoic acid, 4-nitro, 1-methylpropyll ester
Inchi:	InChI=1S/C11H13NO4/c1-3-8(2)16-11(13)9-4-6-10(7-5-9)12(14)15/h4-8H,3H2,1-2H3
InchiKey:	OQECQIDEZLGVDR-UHFFFAOYSA-N
Formula:	C11H13NO4
SMILES:	CCC(C)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	223.23
CAS:	39994-84-8

Physical Properties

Property code	Value	Unit	Source
gf	-56.29	kJ/mol	Joback Method
hf	-306.15	kJ/mol	Joback Method
hfus	28.52	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.550		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1633.00		NIST Webbook
ripol	2368.00		NIST Webbook
ripol	2382.00		NIST Webbook
ripol	2413.00		NIST Webbook
ripol	2353.00		NIST Webbook
ripol	2353.00		NIST Webbook
tb	710.43	K	Joback Method
tc	947.65	K	Joback Method
tf	453.44	K	Joback Method
vc	0.643	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39994848&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume