n-Butyl 4-nitrobenzoate

Other names: Benzoic acid, 4-nitro-, butyl ester
Butyl 4-nitrobenzoate
4-Nitrobenzoic acid, butyl ester
Inchi: InChI=1S/C11H13NO4/c1-2-3-8-16-11(13)9-4-6-10(7-5-9)12(14)15/h4-7H,2-3,8H2,1H3
InchiKey: DVTGVOHTTDVRJF-UHFFFAOYSA-N
Formula: C11H13NO4
SMILES: CCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 223.23
CAS: 120-48-9

Physical Properties

Property code	Value	Unit	Source
gf	-53.85	kJ/mol	Joback Method
hf	-300.87	kJ/mol	Joback Method
hfus	32.05	kJ/mol	Joback Method
hvap	68.77	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.552		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1697.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1697.00		NIST Webbook
rinpol	1738.00		NIST Webbook
ripol	2511.00		NIST Webbook
ripol	2474.00		NIST Webbook
ripol	2472.00		NIST Webbook
ripol	2474.00		NIST Webbook
ripol	2524.00		NIST Webbook
ripol	2472.00		NIST Webbook
tb	710.87	K	Joback Method
tc	943.55	K	Joback Method
tf	468.44	K	Joback Method

vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.69	J/mol×K	710.87	Joback Method
cpg	458.43	J/mol×K	749.65	Joback Method
cpg	470.23	J/mol×K	788.43	Joback Method
cpg	481.10	J/mol×K	827.21	Joback Method
cpg	491.07	J/mol×K	865.99	Joback Method
cpg	500.18	J/mol×K	904.77	Joback Method
cpg	508.44	J/mol×K	943.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	1.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120489&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume