Butyl 3-nitrobenzoate

Other names: Benzoic acid, 3-nitro-, butyl ester
n-Butyl 3-nitrobenzoate
Inchi: InChI=1S/C11H13NO4/c1-2-3-7-16-11(13)9-5-4-6-10(8-9)12(14)15/h4-6,8H,2-3,7H2,1H3
InchiKey: ZJNPXOPNHRBFIP-UHFFFAOYSA-N
Formula: C11H13NO4
SMILES: CCCCOC(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 223.23
CAS: 6268-25-3

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	1766.00		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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6268253&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume