

P-nitro carbanilic acid, n-butyl ester

Inchi:	InChI=1S/C11H14N2O4/c1-2-3-8-17-11(14)12-9-4-6-10(7-5-9)13(15)16/h4-7H,2-3,8H2,1
InchiKey:	FWMIXGBPRUFSQN-UHFFFAOYSA-N
Formula:	C11H14N2O4
SMILES:	CCCCOC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	238.24
CAS:	87457-99-6

Physical Properties

Property code	Value	Unit	Source
gf	35.54	kJ/mol	Joback Method
hf	-247.40	kJ/mol	Joback Method
hfus	37.14	kJ/mol	Joback Method
hvap	75.20	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.943		Crippen Method
mvol	176.930	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
tb	761.04	K	Joback Method
tc	991.73	K	Joback Method
tf	521.10	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.26	J/molxK	761.04	Joback Method
cpg	507.43	J/molxK	799.49	Joback Method
cpg	518.64	J/molxK	837.94	Joback Method
cpg	528.91	J/molxK	876.38	Joback Method
cpg	538.27	J/molxK	914.83	Joback Method
cpg	546.74	J/molxK	953.28	Joback Method
cpg	554.37	J/molxK	991.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C87457996&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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