

Benzoic acid, 4-nitro, 4-pentenyl ester

Other names:	4-Pentenyl 4-nitrobenzoate
Inchi:	InChI=1S/C12H13NO4/c1-2-3-4-9-17-12(14)10-5-7-11(8-6-10)13(15)16/h2,5-8H,1,3-4,9H
InchiKey:	UFYGZXVKAMZTBH-UHFFFAOYSA-N
Formula:	C12H13NO4
SMILES:	<chem>C=CCCCOC(=O)c1ccc([N+](=O)[O-])cc1</chem>
Mol. weight [g/mol]:	235.24

Physical Properties

Property code	Value	Unit	Source
gf	42.41	kJ/mol	Joback Method
hf	-196.08	kJ/mol	Joback Method
hfus	33.36	kJ/mol	Joback Method
hvap	70.32	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.718		Crippen Method
mcpol	176.740	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1793.00		NIST Webbook
rinpol	1804.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1783.00		NIST Webbook
ripol	2662.00		NIST Webbook
ripol	2638.00		NIST Webbook
ripol	2684.00		NIST Webbook
ripol	2642.00		NIST Webbook
tb	730.43	K	Joback Method
tc	963.14	K	Joback Method
tf	477.95	K	Joback Method
vc	0.686	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.28	J/mol×K	730.43	Joback Method

cpg	485.87	J/mol×K	769.21	Joback Method
cpg	497.50	J/mol×K	808.00	Joback Method
cpg	508.20	J/mol×K	846.78	Joback Method
cpg	518.01	J/mol×K	885.57	Joback Method
cpg	526.96	J/mol×K	924.35	Joback Method
cpg	535.09	J/mol×K	963.14	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=R34753&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
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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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