Benzoic acid, 4-nitro-, pentyl ester

Other names:	Amyl p-nitrobenzoate
	4-Nitrobenzoic acid, pentyl ester
	pentyl 4-nitrobenzoate
Inchi:	InChI=1S/C12H15NO4/c1-2-3-4-9-17-12(14)10-5-7-11(8-6-10)13(15)16/h5-8H,2-4,9H2,1
InchiKey:	BFKGHSXQYBELBN-UHFFFAOYSA-N
Formula:	C12H15NO4
SMILES:	CCCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	237.25
CAS:	14309-42-3

Physical Properties

Property code	Value	Unit	Source
gf	-45.43	kJ/mol	Joback Method
hf	-321.51	kJ/mol	Joback Method
hfus	34.64	kJ/mol	Joback Method
hvap	70.99	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	2.942		Crippen Method
mcvol	181.040	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1839.00		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2572.00		NIST Webbook
ripol	2606.00		NIST Webbook
ripol	2582.00		NIST Webbook
tb	733.75	K	Joback Method
tc	962.21	K	Joback Method
tf	479.71	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.53	J/mol×K	733.75	Joback Method
cpg	510.77	J/mol×K	771.83	Joback Method
cpg	523.03	J/mol×K	809.90	Joback Method
cpg	534.34	J/mol×K	847.98	Joback Method
cpg	544.73	J/mol×K	886.06	Joback Method
cpg	554.23	J/mol×K	924.14	Joback Method
cpg	562.86	J/mol×K	962.21	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14309423&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

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