4-Nitrobenzoic acid, 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]: 237.26

Physical Properties

Property code	Value	Unit	Source
af	0.7733		Cheméo Relay (1.0)
hf	-366.21	kJ/mol	Cheméo Relay (1.0)
hfus	34.64	kJ/mol	Joback Method
hvap	90.50	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-4.35		Cheméo Relay (1.0)
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	1805.00		NIST Webbook
rinpol	1799.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1839.00		NIST Webbook
ripol	2582.00		NIST Webbook
ripol	2606.00		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2572.00		NIST Webbook
ripol	2572.00		NIST Webbook
tb	581.66	K	Cheméo Relay (1.0)
tc	815.56	K	Cheméo Relay (1.0)
tf	311.73	K	Cheméo Relay (1.0)
vc	0.657	m3/kmol	Cheméo Relay (1.0)

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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14309423&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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