4-Nitrobenzoic acid, 2-pentyl ester

Other names: Benzoic acid, 4-nitro, 1-methylbutyl ester
Inchi: InChI=1S/C12H15NO4/c1-3-4-9(2)17-12(14)10-5-7-11(8-6-10)13(15)16/h5-9H,3-4H2,1-2
InchiKey: BAJPTXADVLNCKW-UHFFFAOYSA-N
Formula: C12H15NO4
SMILES: CCCC(C)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 237.25
CAS: 100391-69-3

Physical Properties

Property code	Value	Unit	Source
gf	-47.87	kJ/mol	Joback Method
hf	-326.79	kJ/mol	Joback Method
hfus	31.11	kJ/mol	Joback Method
hvap	70.60	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	2.940		Crippen Method
mcvol	181.040	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1724.00		NIST Webbook
ripol	2448.00		NIST Webbook
ripol	2438.00		NIST Webbook
ripol	2438.00		NIST Webbook
ripol	2490.00		NIST Webbook
ripol	2463.00		NIST Webbook
ripol	2448.00		NIST Webbook
tb	733.31	K	Joback Method
tc	966.01	K	Joback Method
tf	464.71	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.12	J/mol×K	733.31	Joback Method
cpg	511.61	J/mol×K	772.09	Joback Method
cpg	524.08	J/mol×K	810.88	Joback Method
cpg	535.55	J/mol×K	849.66	Joback Method
cpg	546.05	J/mol×K	888.45	Joback Method
cpg	555.62	J/mol×K	927.23	Joback Method
cpg	564.27	J/mol×K	966.01	Joback Method

Sources

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=C100391693&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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