4-Nitrobenzoic acid, hexyl ester

Other names: hexyl 4-nitrobenzoate
Inchi: InChI=1S/C13H17NO4/c1-2-3-4-5-10-18-13(15)11-6-8-12(9-7-11)14(16)17/h6-9H,2-5,10
InchiKey: OFWOUNKHYXUEPI-UHFFFAOYSA-N
Formula: C13H17NO4
SMILES: CCCCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 251.28
CAS: 6268-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-37.01	kJ/mol	Joback Method
hf	-342.15	kJ/mol	Joback Method
hfus	37.23	kJ/mol	Joback Method
hvap	73.22	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.332		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	1907.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
ripol	2671.00		NIST Webbook
ripol	2671.00		NIST Webbook
ripol	2689.00		NIST Webbook
ripol	2689.00		NIST Webbook
ripol	2719.00		NIST Webbook
ripol	2704.00		NIST Webbook
tb	756.63	K	Joback Method
tc	981.35	K	Joback Method
tf	490.98	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.59	J/mol×K	756.63	Joback Method
cpg	564.24	J/mol×K	794.08	Joback Method
cpg	576.89	J/mol×K	831.54	Joback Method
cpg	588.56	J/mol×K	868.99	Joback Method
cpg	599.29	J/mol×K	906.44	Joback Method
cpg	609.11	J/mol×K	943.90	Joback Method
cpg	618.06	J/mol×K	981.35	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6268242&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