P-nitro carbanilic acid, n-hexyl ester

Other names: Hexyl N-(4-nitrophenyl) carbamate
Inchi: InChI=1S/C13H18N2O4/c1-2-3-4-5-10-19-13(16)14-11-6-8-12(9-7-11)15(17)18/h6-9H,2-
InchiKey: OFSOQJSHCDPUIU-UHFFFAOYSA-N
Formula: C13H18N2O4
SMILES: CCCCCCOC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 266.29
CAS: 87458-01-3

Physical Properties

Property code	Value	Unit	Source
gf	52.38	kJ/mol	Joback Method
hf	-288.68	kJ/mol	Joback Method
hfus	42.32	kJ/mol	Joback Method
hvap	79.65	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.724		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
tb	806.80	K	Joback Method
tc	1030.70	K	Joback Method
tf	543.64	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.79	J/mol×K	806.80	Joback Method
cpg	615.71	J/mol×K	844.12	Joback Method
cpg	627.61	J/mol×K	881.43	Joback Method
cpg	638.54	J/mol×K	918.75	Joback Method
cpg	648.51	J/mol×K	956.07	Joback Method
cpg	657.57	J/mol×K	993.39	Joback Method
cpg	665.75	J/mol×K	1030.70	Joback Method
hfust	32.74	kJ/mol	376.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87458013&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume