p-Nitro carbanilic acid, n-heptyl ester

Other names: Carbamic acid, N-(4-nitrophenyl)-, heptyl ester
Inchi: InChI=1S/C14H20N2O4/c1-2-3-4-5-6-11-20-14(17)15-12-7-9-13(10-8-12)16(18)19/h7-10
InchiKey: PJOBNIUGOZOAFD-UHFFFAOYSA-N
Formula: C14H20N2O4
SMILES: CCCCCCCOC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 280.32
CAS: 92374-99-7

Physical Properties

Property code	Value	Unit	Source
gf	60.80	kJ/mol	Joback Method
hf	-309.32	kJ/mol	Joback Method
hfus	44.91	kJ/mol	Joback Method
hvap	81.88	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.114		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
tb	829.68	K	Joback Method
tc	1051.05	K	Joback Method
tf	554.91	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.10	J/mol×K	829.68	Joback Method
cpg	671.30	J/mol×K	866.57	Joback Method
cpg	683.47	J/mol×K	903.47	Joback Method
cpg	694.64	J/mol×K	940.36	Joback Method
cpg	704.85	J/mol×K	977.26	Joback Method
cpg	714.13	J/mol×K	1014.15	Joback Method
cpg	722.52	J/mol×K	1051.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92374997&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
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