P-nitro carbanilic acid, n-decyl ester

Inchi: InChI=1S/C17H26N2O4/c1-2-3-4-5-6-7-8-9-14-23-17(20)18-15-10-12-16(13-11-15)19(21
InchiKey: LYVUCZOQWJNQEI-UHFFFAOYSA-N
Formula: C17H26N2O4
SMILES: CCCCCCCCCCOC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 322.40
CAS: 93814-57-4

Physical Properties

Property code	Value	Unit	Source
gf	86.06	kJ/mol	Joback Method
hf	-371.24	kJ/mol	Joback Method
hfus	52.68	kJ/mol	Joback Method
hvap	88.56	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.284		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
tb	898.32	K	Joback Method
tc	1116.00	K	Joback Method
tf	588.72	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.31	J/mol×K	898.32	Joback Method
cpg	843.19	J/mol×K	934.60	Joback Method
cpg	855.96	J/mol×K	970.88	Joback Method
cpg	867.68	J/mol×K	1007.16	Joback Method
cpg	878.38	J/mol×K	1043.44	Joback Method
cpg	888.12	J/mol×K	1079.72	Joback Method
cpg	896.94	J/mol×K	1116.00	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=C93814574&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume