O-nitro carbanilic acid, 2-hexyl ester

Inchi: InChI=1S/C13H18N2O4/c1-3-4-7-10(2)19-13(16)14-11-8-5-6-9-12(11)15(17)18/h5-6,8-10
InchiKey: OKAIAEGTZMZQOD-UHFFFAOYSA-N
Formula: C13H18N2O4
SMILES: CCCCC(C)OC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 266.29
CAS: 93429-11-9

Physical Properties

Property code	Value	Unit	Source
gf	49.94	kJ/mol	Joback Method
hf	-293.96	kJ/mol	Joback Method
hfus	38.80	kJ/mol	Joback Method
hvap	79.27	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.722		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
tb	806.36	K	Joback Method
tc	1033.77	K	Joback Method
tf	528.64	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.38	J/mol×K	806.36	Joback Method
cpg	616.49	J/mol×K	844.26	Joback Method
cpg	628.54	J/mol×K	882.16	Joback Method
cpg	639.57	J/mol×K	920.06	Joback Method
cpg	649.61	J/mol×K	957.97	Joback Method
cpg	658.69	J/mol×K	995.87	Joback Method
cpg	666.85	J/mol×K	1033.77	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93429119&Units=SI

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