M-nitro carbanilic acid, n-nonyl ester

Inchi: InChI=1S/C16H24N2O4/c1-2-3-4-5-6-7-8-12-22-16(19)17-14-10-9-11-15(13-14)18(20)21
InchiKey: XICZRWBYSUBSNJ-UHFFFAOYSA-N
Formula: C16H24N2O4
SMILES: CCCCCCCCCOC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 308.37
CAS: 94373-83-8

Physical Properties

Property code	Value	Unit	Source
gf	77.64	kJ/mol	Joback Method
hf	-350.60	kJ/mol	Joback Method
hfus	50.09	kJ/mol	Joback Method
hvap	86.33	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.894		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
tb	875.44	K	Joback Method
tc	1093.65	K	Joback Method
tf	577.45	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.42	J/mol×K	875.44	Joback Method
cpg	785.09	J/mol×K	911.81	Joback Method
cpg	797.69	J/mol×K	948.18	Joback Method
cpg	809.25	J/mol×K	984.55	Joback Method
cpg	819.81	J/mol×K	1020.92	Joback Method
cpg	829.43	J/mol×K	1057.28	Joback Method
cpg	838.13	J/mol×K	1093.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94373838&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume