

O-nitro carbanilic acid, n-nonyl ester

Inchi:	InChI=1S/C16H24N2O4/c1-2-3-4-5-6-7-10-13-22-16(19)17-14-11-8-9-12-15(14)18(20)21
InchiKey:	LIUBKSDVODUMRW-UHFFFAOYSA-N
Formula:	C16H24N2O4
SMILES:	CCCCCCCCCOC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	308.37
CAS:	94373-84-9

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/molxK	875.44	Joback Method
cpg	785.09	J/molxK	911.81	Joback Method
cpg	797.69	J/molxK	948.18	Joback Method
cpg	809.25	J/molxK	984.55	Joback Method
cpg	819.81	J/molxK	1020.92	Joback Method
cpg	829.43	J/molxK	1057.28	Joback Method
cpg	838.13	J/molxK	1093.65	Joback Method

Sources

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=C94373849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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