

M-nitro carbanilic acid, n-decyl ester

Inchi:	InChI=1S/C17H26N2O4/c1-2-3-4-5-6-7-8-9-13-23-17(20)18-15-11-10-12-16(14-15)19(21)
InchiKey:	BENPOWIZFKFHGE-UHFFFAOYSA-N
Formula:	C17H26N2O4
SMILES:	CCCCCCCCCOC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	322.40
CAS:	94861-52-6

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/molxK	898.32	Joback Method
cpg	843.19	J/molxK	934.60	Joback Method
cpg	855.96	J/molxK	970.88	Joback Method
cpg	867.68	J/molxK	1007.16	Joback Method
cpg	878.38	J/molxK	1043.44	Joback Method
cpg	888.12	J/molxK	1079.72	Joback Method
cpg	896.94	J/molxK	1116.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C94861526&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
mccvol:	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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