

M-nitro carbanilic acid, n-octyl ester

Inchi:	InChI=1S/C15H22N2O4/c1-2-3-4-5-6-7-11-21-15(18)16-13-9-8-10-14(12-13)17(19)20/h8
InchiKey:	XZAZXUURXRVFGJ-UHFFFAOYSA-N
Formula:	C15H22N2O4
SMILES:	CCCCCCCCOC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	294.35
CAS:	94205-20-6

Physical Properties

Property code	Value	Unit	Source
gf	69.22	kJ/mol	Joback Method
hf	-329.96	kJ/mol	Joback Method
hfus	47.50	kJ/mol	Joback Method
hvap	84.11	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.504		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
tb	852.56	K	Joback Method
tc	1072.02	K	Joback Method
tf	566.18	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.33	J/mol×K	852.56	Joback Method
cpg	727.78	J/mol×K	889.14	Joback Method
cpg	740.18	J/mol×K	925.71	Joback Method
cpg	751.56	J/mol×K	962.29	Joback Method
cpg	761.96	J/mol×K	998.87	Joback Method
cpg	771.42	J/mol×K	1035.44	Joback Method
cpg	779.98	J/mol×K	1072.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94205206&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

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