Benzeneacetonitrile, «alpha»-[(1,3-dioxolan-2-ylmethoxy)imino]-

Other names: CGA 92194
Concep ii
«alpha»-((1,3-Dioxolan-2-ylmethoxy)imino)benzeneacetonitrile
Oxabetrinil
N-(1,3-Dioxolan-2-ylmethoxy)benzimidoyl cyanide

Inchi: InChI=1S/C12H12N2O3/c13-8-11(10-4-2-1-3-5-10)14-17-9-12-15-6-7-16-12/h1-5,12H,6-

InchiKey: WFVUIONFJOAYPK-UHFFFAOYSA-N

Formula: C12H12N2O3

SMILES: N#CC(=NOCC1OCCO1)c1ccccc1

Mol. weight [g/mol]: 232.24

CAS: 74782-23-3

Physical Properties

Property code	Value	Unit	Source
hf	-152.91	kJ/mol	Joback Method
hvap	70.14	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.304		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	1921.00		NIST Webbook
tb	770.88	K	Joback Method
tc	1023.95	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74782233&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

hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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