

2-Octyl nitrite

Inchi: InChI=1S/C8H17NO2/c1-3-4-5-6-7-8(2)11-9-10/h8H,3-7H2,1-2H3
InchiKey: WQDGUYZIAJLAB-UHFFFAOYSA-N
Formula: C8H17NO2
SMILES: CCCCCC(C)ON=O
Mol. weight [g/mol]: 159.23

Physical Properties

Property code	Value	Unit	Source
hf	-514.14	kJ/mol	Joback Method
hvap	44.52	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.043		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
ripol	1115.00		NIST Webbook
tb	467.82	K	Joback Method
tc	636.88	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R311509&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
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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