

Octane, 1-azido-

Other names:	1-azidooctane octyl azide
Inchi:	InChI=1S/C8H17N3/c1-2-3-4-5-6-7-8-10-11-9/h2-8H2,1H3
InchiKey:	RXAHCVNYRABXLO-UHFFFAOYSA-N
Formula:	C8H17N3
SMILES:	CCCCCCCCN=[N+]=[N-]
Mol. weight [g/mol]:	155.24
CAS:	7438-05-3

Physical Properties

Property code	Value	Unit	Source
chl	-5674.00 ± 3.00	kJ/mol	NIST Webbook
hfl	96.70	kJ/mol	NIST Webbook
log10ws	-8.26		Crippen Method
logp	3.657		Crippen Method
mcvol	144.920	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rho1	840.00	kg/m3	293.00	Thermochemistry of organic azides revisited

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of organic azides revisited:	https://www.doi.org/10.1016/j.tca.2014.10.015
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7438053&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
hfl:	Liquid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rho:	Liquid Density

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<https://www.chemeo.com/cid/26-057-0/Octane-1-azido.pdf>

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