Benzene, (azidomethyl)-

Other names:	Toluene, «alpha»-azido- «alpha»-Azidotoluene (Azidomethyl)benzene Benzyl azide Toluene, alpha-triazo-
Inchi:	InChI=1S/C7H7N3/c8-10-9-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	UDLLFLQFQMACJB-UHFFFAOYSA-N
Formula:	C7H7N3
SMILES:	[N-]=[N+]=NCc1ccccc1
Mol. weight [g/mol]:	133.15
CAS:	622-79-7

Physical Properties

Property code	Value	Unit	Source
chl	-4123.00 ± 1.00	kJ/mol	NIST Webbook
hf	416.00 ± 2.00	kJ/mol	NIST Webbook
hfl	368.00 ± 1.00	kJ/mol	NIST Webbook
hvap	48.10 ± 0.40	kJ/mol	NIST Webbook
hvap	48.00	kJ/mol	NIST Webbook
log10ws	-7.44		Crippen Method
logp	2.497		Crippen Method
mcvol	107.070	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	48.00	kJ/mol	348.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	356.50 ± 1.50	K	2.10	NIST Webbook
tbrp	381.00	K	3.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C622797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure