

1-Ethynylcyclooctanol

Other names:	Cyclooctanol, 1-ethynyl- 1-Aethinyl-cyclooctanol-(1) 1-Ethynylcyclooctanol
Inchi:	InChI=1S/C10H16O/c1-2-10(11)8-6-4-3-5-7-9-10/h1,11H,3-9H2
InchiKey:	DHAPUKCAOFQTIT-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	C#CC1(O)CCCCCCC1
Mol. weight [g/mol]:	152.24

Physical Properties

Property code	Value	Unit	Source
hfus	10.06	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Cheméo Relay (1.0)
ie	9.91	eV	Cheméo Relay (1.0)
logp	2.095		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
tb	495.44	K	Cheméo Relay (1.0)
tf	329.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.58	J/mol×K	538.83	Joback Method
cpg	348.47	J/mol×K	575.83	Joback Method
cpg	364.26	J/mol×K	612.82	Joback Method
cpg	379.07	J/mol×K	649.82	Joback Method
cpg	392.99	J/mol×K	686.81	Joback Method
cpg	406.16	J/mol×K	723.81	Joback Method
cpg	418.69	J/mol×K	760.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.00 ± 1.00	K	1.60	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55373767&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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