

3-Methyl-1-hexyn-3-ol

Other names:	3-Methyl-1-hexyne-3-ol 3-Methyl-hexin-(1)-ol-(3) Methylpropylethynylcarbinol
Inchi:	InChI=1S/C7H12O/c1-4-6-7(3,8)5-2/h2,8H,4,6H2,1,3H3
InchiKey:	DTGUZRPEDLHAAO-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	C#CC(C)(O)CCC
Mol. weight [g/mol]:	112.17
CAS:	4339-05-3

Physical Properties

Property code	Value	Unit	Source
hfus	13.53	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Cheméo Relay (1.0)
ie	10.14	eV	Cheméo Relay (1.0)
log10ws	-0.89		Cheméo Relay (1.0)
logp	1.171		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
tb	409.65 ± 3.00	K	NIST Webbook
tc	586.88	K	Cheméo Relay (1.0)
tf	233.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.13	J/mol×K	438.63	Joback Method
cpg	231.34	J/mol×K	468.89	Joback Method
cpg	240.97	J/mol×K	499.15	Joback Method
cpg	250.06	J/mol×K	529.41	Joback Method
cpg	258.64	J/mol×K	559.67	Joback Method
cpg	266.72	J/mol×K	589.93	Joback Method
cpg	274.35	J/mol×K	620.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64653e+01
Coeff. B	-4.20115e+03
Coeff. C	-5.50330e+01
Temperature range (K), min.	315.15
Temperature range (K), max.	432.15

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4339053&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

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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