

5-Octyn-3-ol

Inchi:	InChI=1S/C8H14O/c1-3-5-6-7-8(9)4-2/h8-9H,3-4,7H2,1-2H3
InchiKey:	GGXQZVKQXYOPTF-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CCC#CCC(O)CC
Mol. weight [g/mol]:	126.20
CAS:	53723-18-5

Physical Properties

Property code	Value	Unit	Source
gf	80.02	kJ/mol	Joback Method
hf	-93.66	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	51.84	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.561		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	483.18	K	Joback Method
tc	666.51	K	Joback Method
tf	331.84	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.53	J/mol×K	483.18	Joback Method
cpg	269.41	J/mol×K	513.74	Joback Method
cpg	279.84	J/mol×K	544.29	Joback Method
cpg	289.83	J/mol×K	574.85	Joback Method
cpg	299.39	J/mol×K	605.40	Joback Method
cpg	308.54	J/mol×K	635.96	Joback Method
cpg	317.29	J/mol×K	666.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.00	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63973e+01
Coeff. B	-4.75406e+03
Coeff. C	-7.38950e+01
Temperature range (K), min.	369.15
Temperature range (K), max.	503.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53723185&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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