1-Octyn-3-ol, 4-ethyl-

Other names: 4-Ethyl-1-octyn-3-ol
4-ethyloct-1-yn-3-ol
Inchi: InChI=1S/C10H18O/c1-4-7-8-9(5-2)10(11)6-3/h3,9-11H,4-5,7-8H2,1-2H3
InchiKey: CUUQUEAUUPYEKK-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C#CC(O)C(CC)CCCC
Mol. weight [g/mol]: 154.25
CAS: 5877-42-9

Physical Properties

Property code	Value	Unit	Source
gf	114.69	kJ/mol	Joback Method
hf	-120.62	kJ/mol	Joback Method
hfus	21.67	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.197		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	509.62	K	Joback Method
tc	683.63	K	Joback Method
tf	280.25	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.35	J/mol×K	509.62	Joback Method
cpg	358.04	J/mol×K	538.62	Joback Method
cpg	370.16	J/mol×K	567.62	Joback Method
cpg	381.74	J/mol×K	596.62	Joback Method
cpg	392.79	J/mol×K	625.63	Joback Method
cpg	403.34	J/mol×K	654.63	Joback Method
cpg	413.41	J/mol×K	683.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	404.00 ± 1.00	K	7.90	NIST Webbook
tbrp	364.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63622e+01
Coeff. B	-5.10696e+03
Coeff. C	-8.59310e+01
Temperature range (K), min.	403.15
Temperature range (K), max.	548.15

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=C5877429&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