6-Octen-1-yn-3-ol, 3,7-dimethyl-

Other names:	3,7-Dimethyl-6-octen-1-yn-3-ol
	2,7-Dimethyl-7-octen-5-yn-4-ol
	Dehydrolinalool
	Linalool, dehydro-
	Dehydro-«beta»-linalool
	3,7-dimethyloct-6-en-1-yn-3-ol
Inchi:	InChI=1S/C10H16O/c1-5-10(4,11)8-6-7-9(2)3/h1,7,11H,6,8H2,2-4H3
InchiKey:	YWTIDNZYLFTNQQ-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	C#CC(C)(O)CCC=C(C)C
Mol. weight [g/mol]:	152.23
CAS:	29171-20-8

Physical Properties

Property code	Value	Unit	Source
gf	194.08	kJ/mol	Joback Method
hf	-11.38	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	53.13	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.117		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1068.40		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
ripol	1617.00		NIST Webbook
tb	511.31	K	Joback Method
tc	699.12	K	Joback Method
tf	293.63	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.17	J/mol×K	511.31	Joback Method
cpg	342.88	J/mol×K	542.61	Joback Method
cpg	354.83	J/mol×K	573.91	Joback Method
cpg	366.08	J/mol×K	605.21	Joback Method
cpg	376.66	J/mol×K	636.51	Joback Method
cpg	386.63	J/mol×K	667.81	Joback Method
cpg	396.04	J/mol×K	699.12	Joback Method
cpl	385.20	J/mol×K	313.55	NIST Webbook
hvapt	52.10	kJ/mol	438.50	NIST Webbook
hvapt	50.40 ± 0.10	kJ/mol	407.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C29171208&Units=SI

Legend

cpg: Ideal gas heat capacity
cpl: Liquid phase 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
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
pc: Critical Pressure
rinpol: Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume