

1,7-Octadien-3-ol, 2,6-dimethyl-

Other names:	3,7-Dimethyl-1, 7-octadien-6-ol 2,6-Dimethyl-1,7-octadien-3-ol 2,3-Dimethyl-1,7-octadien-3-ol
Inchi:	InChI=1S/C10H18O/c1-5-9(4)6-7-10(11)8(2)3/h5,9-11H,1-2,6-7H2,3-4H3
InchiKey:	TYASLDPXCAROPT-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=CC(C)CCC(O)C(=C)C
Mol. weight [g/mol]:	154.25
CAS:	22460-59-9

Physical Properties

Property code	Value	Unit	Source
gf	58.75	kJ/mol	Joback Method
hf	-171.45	kJ/mol	Joback Method
hfus	14.83	kJ/mol	Joback Method
hvap	52.50	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.526		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
tb	512.74	K	Joback Method
tc	685.52	K	Joback Method
tf	215.80	K	Joback Method
vc	0.566	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.62	J/mol×K	512.74	Joback Method
cpg	356.56	J/mol×K	541.54	Joback Method
cpg	368.90	J/mol×K	570.33	Joback Method
cpg	380.68	J/mol×K	599.13	Joback Method

cpg	391.92	J/mol×K	627.93	Joback Method
cpg	402.63	J/mol×K	656.73	Joback Method
cpg	412.83	J/mol×K	685.52	Joback Method

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=C22460599&Units=SI
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
hvac:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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