

1,5-Heptadien-4-ol, 3,3,6-trimethyl-

Other names:	3,3,6-Trimethyl-1,5-heptadien-4-ol 2,5,5-trimethylhepta-2,6-dien-4-ol Artemisia alcohol 3,3,6-Trimethylhepta-1,5-dien-4-ol (.+/-)-Artemisia alcohol
Inchi:	InChI=1S/C10H18O/c1-6-10(4,5)9(11)7-8(2)3/h6-7,9,11H,1H2,2-5H3
InchiKey:	WPPVSYVQAKQNJK-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=CC(C)(C)C(O)C=C(C)C
Mol. weight [g/mol]:	154.25
CAS:	27644-04-8

Physical Properties

Property code	Value	Unit	Source
gf	56.41	kJ/mol	Joback Method
hf	-183.13	kJ/mol	Joback Method
hfus	12.42	kJ/mol	Joback Method
hvap	52.22	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.526		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1068.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1071.80		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1085.30		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1083.00		NIST Webbook

rinpol	1081.00	NIST Webbook
rinpol	1081.00	NIST Webbook
rinpol	1069.00	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1066.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1064.00	NIST Webbook
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rinpol	1083.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1079.00	NIST Webbook
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rinpol	1074.00	NIST Webbook
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rinpol	1079.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1083.00	NIST Webbook
rinpol	1070.00	NIST Webbook
ripol	1523.00	NIST Webbook
ripol	1478.00	NIST Webbook
ripol	1476.00	NIST Webbook
ripol	1515.00	NIST Webbook
ripol	1495.00	NIST Webbook
ripol	1509.00	NIST Webbook

ripol	1510.00		NIST Webbook
ripol	1511.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1510.00		NIST Webbook
tb	517.43	K	Joback Method
tc	700.79	K	Joback Method
tf	229.90	K	Joback Method
vc	0.559	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.28	J/molxK	517.43	Joback Method
cpg	360.97	J/molxK	547.99	Joback Method
cpg	373.89	J/molxK	578.55	Joback Method
cpg	386.07	J/molxK	609.11	Joback Method
cpg	397.57	J/molxK	639.67	Joback Method
cpg	408.42	J/molxK	670.23	Joback Method
cpg	418.68	J/molxK	700.79	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C27644048&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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