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	1076.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1065.00		NIST Webbook

rinpol	1083.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1084.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1079.00	NIST Webbook
rinpol	1089.00	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1083.00	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	1070.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1083.00	NIST Webbook
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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	1084.00	NIST Webbook
ripol	1510.00	NIST Webbook
ripol	1515.00	NIST Webbook
ripol	1510.00	NIST Webbook
ripol	1478.00	NIST Webbook
ripol	1515.00	NIST Webbook
ripol	1495.00	NIST Webbook

ripol	1488.00		NIST Webbook
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ripol	1511.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1476.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1523.00		NIST Webbook
tb	517.43	K	Joback Method
tc	700.79	K	Joback Method
tf	229.90	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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

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

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
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

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