3,3,6-Trimethyl-1,4-heptadien-6-ol

Other names: Yomogi alcohol
Inchi: InChI=1S/C10H18O/c1-6-9(2,3)7-8-10(4,5)11/h6-8,11H,1H2,2-5H3/b8-7+
InchiKey: CSMMFGCGBLZIJE-BQYQJAHWSA-N
Formula: C10H18O
SMILES: C=CC(C)(C)C=CC(C)(C)O
Mol. weight [g/mol]: 154.25
CAS: 30458-12-9

Physical Properties

Property code	Value	Unit	Source
gf	70.24	kJ/mol	Joback Method
hf	-176.81	kJ/mol	Joback Method
hfus	9.84	kJ/mol	Joback Method
hvap	51.23	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.526		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	998.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	998.00		NIST Webbook

rinpol	987.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	999.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1377.00		NIST Webbook
tb	514.76	K	Joback Method
tc	701.77	K	Joback Method
tf	261.28	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.28	J/mol×K	514.76	Joback Method
cpg	364.41	J/mol×K	545.93	Joback Method
cpg	377.62	J/mol×K	577.10	Joback Method
cpg	389.99	J/mol×K	608.27	Joback Method

cpg	401.58	J/mol×K	639.43	Joback Method
cpg	412.43	J/mol×K	670.60	Joback Method
cpg	422.61	J/mol×K	701.77	Joback Method
dvisc	0.0565216	Pa×s	261.28	Joback Method
dvisc	0.0094188	Pa×s	303.53	Joback Method
dvisc	0.0024319	Pa×s	345.77	Joback Method
dvisc	0.0008432	Pa×s	388.02	Joback Method
dvisc	0.0003600	Pa×s	430.27	Joback Method
dvisc	0.0001789	Pa×s	472.51	Joback Method
dvisc	0.0000998	Pa×s	514.76	Joback Method

Sources

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=C30458129&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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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