

trans,trans-2,6-Dimethyl-2,6-octadiene-1,8-diol

Other names:	(E)-8-hydroxygeraniol
Inchi:	InChI=1S/C10H18O2/c1-9(6-7-11)4-3-5-10(2)8-12/h5-6,11-12H,3-4,7-8H2,1-2H3/b9-6+,10-11
InchiKey:	PREUOUJFXMCMMSJ-TXFIJWAUSA-N
Formula:	C10H18O2
SMILES:	CC(=CCCC(C)=CCO)CO
Mol. weight [g/mol]:	170.25
CAS:	26488-97-1

Physical Properties

Property code	Value	Unit	Source
gf	-96.98	kJ/mol	Joback Method
hf	-339.33	kJ/mol	Joback Method
hfus	27.62	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.644		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
ripol	2629.00		NIST Webbook
ripol	2651.00		NIST Webbook
ripol	2652.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2627.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2652.00		NIST Webbook
ripol	2640.00		NIST Webbook
tb	620.64	K	Joback Method
tc	791.70	K	Joback Method
tf	286.02	K	Joback Method
vc	0.596	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	399.38	J/mol×K	620.64	Joback Method
cpg	410.17	J/mol×K	649.15	Joback Method
cpg	420.45	J/mol×K	677.66	Joback Method
cpg	430.24	J/mol×K	706.17	Joback Method
cpg	439.60	J/mol×K	734.68	Joback Method
cpg	448.53	J/mol×K	763.19	Joback Method
cpg	457.08	J/mol×K	791.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26488971&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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