

2H-1-Benzopyran-6-ol, 3,4-dihydro-2,8-dimethyl-2-[(3E,7E)-4,8,12-trimethyl-2H-1-benzopyran-6-yl]-(2R)-

Other names:	Delta-Tocotrienol Tocotrienol, 8-methyl
Inchi:	InChI=1S/C27H40O2/c1-20(2)10-7-11-21(3)12-8-13-22(4)14-9-16-27(6)17-15-24-19-25(2)
InchiKey:	ODADKLYLWWCHNB-NDZYPVAJSA-N
Formula:	C27H40O2
SMILES:	CC(C)=CCCC(C)=CCCC(C)=CCCC1(C)CCc2cc(O)cc(C)c2O1
Mol. weight [g/mol]:	396.61
CAS:	25612-59-3

Physical Properties

Property code	Value	Unit	Source
gf	287.04	kJ/mol	Joback Method
hf	-292.16	kJ/mol	Joback Method
hfus	59.12	kJ/mol	Joback Method
hvap	95.87	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	7.984		Crippen Method
mcvol	355.510	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
rinpol	3072.70		NIST Webbook
rinpol	2985.00		NIST Webbook
rinpol	3072.70		NIST Webbook
rinpol	2985.00		NIST Webbook
tb	984.74	K	Joback Method
tc	1214.90	K	Joback Method
tf	565.00	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.39	J/molxK	984.74	Joback Method
cpg	1242.04	J/molxK	1023.10	Joback Method
cpg	1269.54	J/molxK	1061.46	Joback Method

cpg	1298.21	J/mol×K	1099.82	Joback Method
cpg	1328.37	J/mol×K	1138.18	Joback Method
cpg	1360.32	J/mol×K	1176.54	Joback Method
cpg	1394.38	J/mol×K	1214.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25612593&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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