

2H-1-Benzopyran-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-[(3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl]chroman-6-ol (2R)-

Other names:

Gamma-Tocotrienol

(R)-2,7,8-Trimethyl-2-((3E,7E)-4,8,12-trimethyltrideca-3,7,11-trien-1-yl)chroman-6-ol

Inchi: InChI=1S/C28H42O2/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-28(7)18-16-25-19-26

InchiKey: OTXNTMVVOOBZCV-UXRBPBJUSA-N

Formula: C28H42O2

SMILES: CC(C)=CCCC(C)=CCCC(C)=CCCC1(C)CCc2cc(O)c(C)c(C)c2O1

Mol. weight [g/mol]: 410.63

CAS: 14101-61-2

Physical Properties

Property code	Value	Unit	Source
gf	285.83	kJ/mol	Joback Method
hf	-324.27	kJ/mol	Joback Method
hfus	61.32	kJ/mol	Joback Method
hvap	98.76	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	8.292		Crippen Method
mvol	369.600	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	3170.90		NIST Webbook
rinpol	3170.90		NIST Webbook
tb	1012.60	K	Joback Method
tc	1244.99	K	Joback Method
tf	588.79	K	Joback Method
vc	1.373	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.49	J/molxK	1012.60	Joback Method
cpg	1311.78	J/molxK	1051.33	Joback Method
cpg	1341.08	J/molxK	1090.06	Joback Method
cpg	1371.73	J/molxK	1128.80	Joback Method
cpg	1404.03	J/molxK	1167.53	Joback Method

cpg	1438.31	J/mol×K	1206.26	Joback Method
cpg	1474.89	J/mol×K	1244.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14101612&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
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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