dl-«alpha»-Tocopherol

Other names: (.+/-.)-«alpha»-Tocopherol
2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-
6-Chromanol, 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-
3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-ol
Inchi: InChI=1S/C29H50O2/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-29(8)19-17-26-25(7
InchiKey: GVJHHUAWPYXKBD-UHFFFAOYSA-N
Formula: C29H50O2
SMILES: Cc1c(C)c2c(c(C)c1O)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
Mol. weight [g/mol]: 430.71
CAS: 10191-41-0

Physical Properties

Property code	Value	Unit	Source
gf	62.29	kJ/mol	Joback Method
hf	-694.51	kJ/mol	Joback Method
hfus	56.28	kJ/mol	Joback Method
hvap	100.37	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.840		Crippen Method
mcvol	396.590	ml/mol	McGowan Method
pc	882.09	kPa	Joback Method
rinpol	3149.50		NIST Webbook
rinpol	3149.50		NIST Webbook
tb	1027.02	K	Joback Method
tc	1257.43	K	Joback Method
tf	624.70	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1437.29	J/mol×K	1027.02	Joback Method
cpg	1465.97	J/mol×K	1065.42	Joback Method
cpg	1495.02	J/mol×K	1103.82	Joback Method

cpg	1524.68	J/mol×K	1142.22	Joback Method
cpg	1555.22	J/mol×K	1180.63	Joback Method
cpg	1586.87	J/mol×K	1219.03	Joback Method
cpg	1619.91	J/mol×K	1257.43	Joback Method

Sources

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=C10191410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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