«alpha»-Tocospiro A

Inchi: InChI=1S/C29H50O4/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-17-27(8)18-19-28(33-2
InchiKey: NFNYYDIZCJKCQK-UHFFFAOYSA-N
Formula: C29H50O4
SMILES: CC(=O)C1(O)C(C)=C(C)C(=O)C12CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2
Mol. weight [g/mol]: 462.70
CAS: 601490-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-216.75	kJ/mol	Joback Method
hf	-1004.90	kJ/mol	Joback Method
hfus	46.06	kJ/mol	Joback Method
hvap	109.36	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.973		Crippen Method
mcvol	408.330	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2860.30		NIST Webbook
rinpol	2860.30		NIST Webbook
tb	1133.88	K	Joback Method
tc	1394.56	K	Joback Method
tf	695.71	K	Joback Method
vc	1.563	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1637.03	J/mol×K	1133.88	Joback Method
cpg	1687.54	J/mol×K	1177.33	Joback Method
cpg	1741.87	J/mol×K	1220.77	Joback Method
cpg	1800.60	J/mol×K	1264.22	Joback Method
cpg	1864.28	J/mol×K	1307.67	Joback Method
cpg	1933.47	J/mol×K	1351.11	Joback Method
cpg	2008.74	J/mol×K	1394.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C601490408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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