(Z)-6-Methyl-2-(tricos-14-en-1-yl)-2H-pyran-4(3H)-o

Inchi: InChI=1S/C29H52O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey: DCWXKWMWPSIAIY-KHPPLWFESA-N
Formula: C29H52O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCCCC1CC(=O)C=C(C)O1
Mol. weight [g/mol]: 432.72
CAS: 243118-20-9

Physical Properties

Property code	Value	Unit	Source
gf	109.59	kJ/mol	Joback Method
hf	-693.74	kJ/mol	Joback Method
hfus	71.23	kJ/mol	Joback Method
hvap	90.25	kJ/mol	Joback Method
log10ws	-10.54		Crippen Method
logp	9.626		Crippen Method
mcvol	407.450	ml/mol	McGowan Method
pc	731.25	kPa	Joback Method
rinpol	3353.60		NIST Webbook
rinpol	3353.60		NIST Webbook
tb	985.54	K	Joback Method
tc	1208.13	K	Joback Method
tf	526.96	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1445.49	J/mol×K	985.54	Joback Method
cpg	1467.48	J/mol×K	1022.64	Joback Method
cpg	1487.76	J/mol×K	1059.74	Joback Method
cpg	1506.42	J/mol×K	1096.84	Joback Method
cpg	1523.53	J/mol×K	1133.93	Joback Method
cpg	1539.16	J/mol×K	1171.03	Joback Method
cpg	1553.40	J/mol×K	1208.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C243118209&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