(Z)-2-(henicos-12-en-1-yl)-6-methyl-2H-pyran-4(3H

Inchi: InChI=1S/C27H48O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-27-24-2
InchiKey: SQWASCWUQBNPCS-KHPPLWFESA-N
Formula: C27H48O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCC1CC(=O)C=C(C)O1
Mol. weight [g/mol]: 404.67
CAS: 243118-19-6

Physical Properties

Property code	Value	Unit	Source
gf	92.75	kJ/mol	Joback Method
hf	-652.46	kJ/mol	Joback Method
hfus	66.05	kJ/mol	Joback Method
hvap	85.79	kJ/mol	Joback Method
log10ws	-9.70		Crippen Method
logp	8.846		Crippen Method
mcvol	379.270	ml/mol	McGowan Method
pc	813.53	kPa	Joback Method
rinpol	3146.10		NIST Webbook
rinpol	3146.10		NIST Webbook
tb	939.78	K	Joback Method
tc	1150.60	K	Joback Method
tf	504.42	K	Joback Method
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.51	J/mol×K	939.78	Joback Method
cpg	1336.81	J/mol×K	974.92	Joback Method
cpg	1356.60	J/mol×K	1010.05	Joback Method
cpg	1374.92	J/mol×K	1045.19	Joback Method
cpg	1391.84	J/mol×K	1080.32	Joback Method
cpg	1407.42	J/mol×K	1115.46	Joback Method
cpg	1421.72	J/mol×K	1150.60	Joback Method

Sources

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=C243118196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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