(E)-4-(2-(2-(2,6-Dimethylhepta-1,5-dien-1-yl)-6-pen

Inchi: InChI=1S/C27H42O4/c1-6-7-8-12-23-19-24(15-13-22-14-16-25(28)26(18-22)29-5)31-27(

InchiKey: MJGVDELZBZAFOX-HEHNFIMWSA-N

Formula: C27H42O4

SMILES: CCCCCC1CC(CCc2ccc(O)c(OC)c2)OC(C=C(C)CCC=C(C)C)O1

Mol. weight [g/mol]: 430.62

CAS: 863913-68-2

Physical Properties

Property code	Value	Unit	Source
gf	-0.25	kJ/mol	Joback Method
hf	-720.58	kJ/mol	Joback Method
hfus	74.03	kJ/mol	Joback Method
hvap	102.97	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	7.107		Crippen Method
mcvol	371.550	ml/mol	McGowan Method
pc	1022.69	kPa	Joback Method
rinpol	3105.90		NIST Webbook
rinpol	3105.90		NIST Webbook
tb	1024.05	K	Joback Method
tc	1255.84	K	Joback Method
tf	580.90	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.52	J/mol×K	1024.05	Joback Method
cpg	1340.76	J/mol×K	1062.68	Joback Method
cpg	1360.05	J/mol×K	1101.31	Joback Method
cpg	1378.54	J/mol×K	1139.95	Joback Method
cpg	1396.35	J/mol×K	1178.58	Joback Method
cpg	1413.66	J/mol×K	1217.21	Joback Method
cpg	1430.59	J/mol×K	1255.84	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C863913682&Units=SI

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