Succinic acid, dodec-2-en-1-yl cis-4-methylcyclohexyl ester

Inchi: InChI=1S/C23H40O4/c1-3-4-5-6-7-8-9-10-11-12-19-26-22(24)17-18-23(25)27-21-15-13-2

InchiKey: GAJHXWHTRANSKR-QXMHVHEDSA-N

Formula: C23H40O4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)OC1CCC(C)CC1

Mol. weight [g/mol]: 380.56

Physical Properties

Property code	Value	Unit	Source
gf	-228.10	kJ/mol	Joback Method
hf	-856.45	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.129		Crippen Method
mcvol	334.650	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2732.00		NIST Webbook
rinpol	2732.00		NIST Webbook
tb	897.26	K	Joback Method
tc	1101.43	K	Joback Method
tf	491.35	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.68	J/mol×K	897.26	Joback Method
cpg	1210.37	J/mol×K	1067.40	Joback Method
cpg	1196.75	J/mol×K	1033.37	Joback Method
cpg	1181.81	J/mol×K	999.34	Joback Method
cpg	1165.51	J/mol×K	965.32	Joback Method
cpg	1147.81	J/mol×K	931.29	Joback Method
cpg	1222.71	J/mol×K	1101.43	Joback Method
dvisc	0.0000404	Pa×s	897.26	Joback Method

dvisc	0.0000534	Pa×s	829.61	Joback Method
dvisc	0.0000741	Pa×s	761.96	Joback Method
dvisc	0.0001097	Pa×s	694.31	Joback Method
dvisc	0.0001766	Pa×s	626.65	Joback Method
dvisc	0.0003193	Pa×s	559.00	Joback Method
dvisc	0.0006793	Pa×s	491.35	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=U390062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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