Succinic acid, dodec-2-en-1-yl cyclopentyl ester

Inchi: InChI=1S/C21H36O4/c1-2-3-4-5-6-7-8-9-10-13-18-24-20(22)16-17-21(23)25-19-14-11-12

InchiKey: CPJMJTNJHCAPJD-JLHYYAGUSA-N

Formula: C21H36O4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)OC1CCCC1

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-225.13	kJ/mol	Joback Method
hf	-788.67	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.492		Crippen Method
mcvol	306.470	ml/mol	McGowan Method
pc	1180.90	kPa	Joback Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook
tb	851.90	K	Joback Method
tc	1049.79	K	Joback Method
tf	476.57	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.03	J/mol×K	851.90	Joback Method
cpg	1077.44	J/mol×K	1016.81	Joback Method
cpg	1063.56	J/mol×K	983.83	Joback Method
cpg	1048.62	J/mol×K	950.85	Joback Method
cpg	1032.58	J/mol×K	917.86	Joback Method
cpg	1015.40	J/mol×K	884.88	Joback Method
cpg	1090.30	J/mol×K	1049.79	Joback Method
dvisc	0.0000598	Pa×s	851.90	Joback Method

dvisc	0.0000784	Pa×s	789.35	Joback Method
dvisc	0.0001077	Pa×s	726.79	Joback Method
dvisc	0.0001571	Pa×s	664.24	Joback Method
dvisc	0.0002478	Pa×s	601.68	Joback Method
dvisc	0.0004344	Pa×s	539.12	Joback Method
dvisc	0.0008826	Pa×s	476.57	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=U391385&Units=SI

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