Succinic acid, dec-2-yl 4-(4-methoxyphenyl)cyclohexyl ester

Inchi: InChI=1S/C27H42O5/c1-4-5-6-7-8-9-10-21(2)31-26(28)19-20-27(29)32-25-17-13-23(14-1

InchiKey: CJNDZFWCIJKSPC-UHFFFAOYSA-N

Formula: C27H42O5

SMILES: CCCCCCCCC(C)OC(=O)CCC(=O)OC1CCC(c2ccc(OC)cc2)CC1

Mol. weight [g/mol]: 446.62

Physical Properties

Property code	Value	Unit	Source
gf	-279.30	kJ/mol	Joback Method
hf	-968.67	kJ/mol	Joback Method
hfus	55.48	kJ/mol	Joback Method
hvap	99.09	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.727		Crippen Method
mcvol	377.420	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	3326.00		NIST Webbook
rinpol	3326.00		NIST Webbook
tb	1038.26	K	Joback Method
tc	1271.13	K	Joback Method
tf	587.68	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1333.76	J/mol×K	1038.26	Joback Method
cpg	1349.07	J/mol×K	1077.07	Joback Method
cpg	1362.22	J/mol×K	1115.88	Joback Method
cpg	1373.26	J/mol×K	1154.69	Joback Method
cpg	1382.21	J/mol×K	1193.50	Joback Method
cpg	1389.13	J/mol×K	1232.31	Joback Method
cpg	1394.05	J/mol×K	1271.13	Joback Method
dvisc	0.0002602	Pa×s	587.68	Joback Method

dvisc	0.0001298	Pa×s	662.78	Joback Method
dvisc	0.0000746	Pa×s	737.87	Joback Method
dvisc	0.0000475	Pa×s	812.97	Joback Method
dvisc	0.0000326	Pa×s	888.07	Joback Method
dvisc	0.0000238	Pa×s	963.16	Joback Method
dvisc	0.0000181	Pa×s	1038.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390042&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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