Succinic acid, 2-methylpent-3-yl 4-(4-methoxyphenyl)cyclohexyl ester

Inchi: InChI=1S/C23H34O5/c1-5-21(16(2)3)28-23(25)15-14-22(24)27-20-12-8-18(9-13-20)17-6

InchiKey: ACBJWYYLOXMMJH-UHFFFAOYSA-N

Formula: C23H34O5

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

Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-315.42	kJ/mol	Joback Method
hf	-891.39	kJ/mol	Joback Method
hfus	41.60	kJ/mol	Joback Method
hvap	89.80	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.023		Crippen Method
mcvol	321.060	ml/mol	McGowan Method
pc	1233.74	kPa	Joback Method
rinpol	2919.00		NIST Webbook
rinpol	2919.00		NIST Webbook
tb	946.30	K	Joback Method
tc	1168.73	K	Joback Method
tf	527.60	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.87	J/mol×K	946.30	Joback Method
cpg	1104.05	J/mol×K	983.37	Joback Method
cpg	1118.38	J/mol×K	1020.44	Joback Method
cpg	1130.87	J/mol×K	1057.51	Joback Method
cpg	1141.56	J/mol×K	1094.59	Joback Method
cpg	1150.44	J/mol×K	1131.66	Joback Method
cpg	1157.56	J/mol×K	1168.73	Joback Method
dvisc	0.0004670	Pa×s	527.60	Joback Method

dvisc	0.0002264	Pa×s	597.38	Joback Method
dvisc	0.0001277	Pa×s	667.17	Joback Method
dvisc	0.0000803	Pa×s	736.95	Joback Method
dvisc	0.0000547	Pa×s	806.73	Joback Method
dvisc	0.0000396	Pa×s	876.52	Joback Method
dvisc	0.0000301	Pa×s	946.30	Joback Method

Sources

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=U390038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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