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

Inchi: InChI=1S/C22H32O5/c1-15(2)16(3)26-21(23)13-14-22(24)27-20-11-7-18(8-12-20)17-5-9

InchiKey: MNPPIGNFBUPNMZ-UHFFFAOYSA-N

Formula: C22H32O5

SMILES: COc1ccc(C2CCC(OC(=O)CCC(=O)OC(C)C(C)C)CC2)cc1

Mol. weight [g/mol]: 376.49

Physical Properties

Property code	Value	Unit	Source
gf	-323.84	kJ/mol	Joback Method
hf	-870.75	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	87.57	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.632		Crippen Method
mcvol	306.970	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2840.00		NIST Webbook
rinpol	2840.00		NIST Webbook
tb	923.42	K	Joback Method
tc	1145.49	K	Joback Method
tf	516.33	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.16	J/mol×K	923.42	Joback Method
cpg	1043.56	J/mol×K	960.43	Joback Method
cpg	1058.17	J/mol×K	997.44	Joback Method
cpg	1070.99	J/mol×K	1034.46	Joback Method
cpg	1082.04	J/mol×K	1071.47	Joback Method
cpg	1091.33	J/mol×K	1108.48	Joback Method
cpg	1098.89	J/mol×K	1145.49	Joback Method
dvisc	0.0005240	Pa×s	516.33	Joback Method

dvisc	0.0002566	Pa×s	584.18	Joback Method
dvisc	0.0001457	Pa×s	652.03	Joback Method
dvisc	0.0000921	Pa×s	719.88	Joback Method
dvisc	0.0000630	Pa×s	787.72	Joback Method
dvisc	0.0000458	Pa×s	855.57	Joback Method
dvisc	0.0000348	Pa×s	923.42	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=U390037&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