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

Inchi: InChI=1S/C24H36O5/c1-4-5-6-7-18(2)28-23(25)16-17-24(26)29-22-14-10-20(11-15-22)1

InchiKey: WYIZBKRKMFEYMG-UHFFFAOYSA-N

Formula: C24H36O5

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

Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-304.56	kJ/mol	Joback Method
hf	-906.75	kJ/mol	Joback Method
hfus	47.71	kJ/mol	Joback Method
hvap	92.41	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.557		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	3031.00		NIST Webbook
rinpol	3031.00		NIST Webbook
tb	969.62	K	Joback Method
tc	1192.03	K	Joback Method
tf	553.87	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.58	J/mol×K	969.62	Joback Method
cpg	1164.49	J/mol×K	1006.69	Joback Method
cpg	1178.52	J/mol×K	1043.76	Joback Method
cpg	1190.70	J/mol×K	1080.83	Joback Method
cpg	1201.05	J/mol×K	1117.89	Joback Method
cpg	1209.59	J/mol×K	1154.96	Joback Method
cpg	1216.34	J/mol×K	1192.03	Joback Method
dvisc	0.0003740	Pa×s	553.87	Joback Method

dvisc	0.0001919	Pa×s	623.16	Joback Method
dvisc	0.0001125	Pa×s	692.45	Joback Method
dvisc	0.0000727	Pa×s	761.74	Joback Method
dvisc	0.0000505	Pa×s	831.04	Joback Method
dvisc	0.0000371	Pa×s	900.33	Joback Method
dvisc	0.0000285	Pa×s	969.62	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=U390039&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