Succinic acid, cyclohexylmethyl 4-(4-methoxyphenyl)cyclohexyl ester

Inchi: InChI=1S/C24H34O5/c1-27-21-11-7-19(8-12-21)20-9-13-22(14-10-20)29-24(26)16-15-23

InchiKey: SVQCUAVNBKCZLT-UHFFFAOYSA-N

Formula: C24H34O5

SMILES: COc1ccc(C2CCC(OC(=O)CCC(=O)OCC3CCCCC3)CC2)cc1

Mol. weight [g/mol]: 402.52

Physical Properties

Property code	Value	Unit	Source
gf	-277.67	kJ/mol	Joback Method
hf	-847.15	kJ/mol	Joback Method
hfus	43.07	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.168		Crippen Method
mcvol	324.290	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	3284.00		NIST Webbook
rinpol	3284.00		NIST Webbook
tb	989.61	K	Joback Method
tc	1225.77	K	Joback Method
tf	576.25	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1142.02	J/mol×K	989.61	Joback Method
cpg	1157.38	J/mol×K	1028.97	Joback Method
cpg	1170.49	J/mol×K	1068.33	Joback Method
cpg	1181.39	J/mol×K	1107.69	Joback Method
cpg	1190.11	J/mol×K	1147.05	Joback Method
cpg	1196.68	J/mol×K	1186.41	Joback Method
cpg	1201.12	J/mol×K	1225.77	Joback Method
dvisc	0.0003819	Pa×s	576.25	Joback Method

dvisc	0.0002029	Pa×s	645.14	Joback Method
dvisc	0.0001218	Pa×s	714.04	Joback Method
dvisc	0.0000800	Pa×s	782.93	Joback Method
dvisc	0.0000562	Pa×s	851.82	Joback Method
dvisc	0.0000417	Pa×s	920.72	Joback Method
dvisc	0.0000322	Pa×s	989.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390041&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