Succinic acid, 4-phenoxybenzyl tridecyl ester

Inchi: InChI=1S/C30H42O5/c1-2-3-4-5-6-7-8-9-10-11-15-24-33-29(31)22-23-30(32)34-25-26-18
InchiKey: AFHPHNTUQBEXEG-UHFFFAOYSA-N
Formula: C30H42O5
SMILES: CCCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 482.65

Physical Properties

Property code	Value	Unit	Source
gf	-155.93	kJ/mol	Joback Method
hf	-822.76	kJ/mol	Joback Method
hfus	67.91	kJ/mol	Joback Method
hvap	108.31	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	8.157		Crippen Method
mcvol	406.790	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	3599.00		NIST Webbook
rinpol	3599.00		NIST Webbook
tb	1119.14	K	Joback Method
tc	1375.85	K	Joback Method
tf	659.77	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.11	J/mol×K	1119.14	Joback Method
cpg	1457.90	J/mol×K	1333.06	Joback Method
cpg	1452.18	J/mol×K	1290.28	Joback Method
cpg	1444.63	J/mol×K	1247.49	Joback Method
cpg	1435.16	J/mol×K	1204.71	Joback Method
cpg	1423.68	J/mol×K	1161.92	Joback Method
cpg	1461.88	J/mol×K	1375.85	Joback Method
dvisc	0.0000093	Pa×s	1119.14	Joback Method

dvisc	0.0000121	Pa×s	1042.58	Joback Method
dvisc	0.0000164	Pa×s	966.02	Joback Method
dvisc	0.0000235	Pa×s	889.45	Joback Method
dvisc	0.0000359	Pa×s	812.89	Joback Method
dvisc	0.0000600	Pa×s	736.33	Joback Method
dvisc	0.0001128	Pa×s	659.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349603&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