Succinic acid, isobutyl 4-phenoxybenzyl ester

Inchi: InChI=1S/C21H24O5/c1-16(2)14-24-20(22)12-13-21(23)25-15-17-8-10-19(11-9-17)26-18
InchiKey: LUVCBMAVBVHVKQ-UHFFFAOYSA-N
Formula: C21H24O5
SMILES: CC(C)COC(=O)CCC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 356.41

Physical Properties

Property code	Value	Unit	Source
gf	-234.15	kJ/mol	Joback Method
hf	-642.28	kJ/mol	Joback Method
hfus	41.08	kJ/mol	Joback Method
hvap	87.89	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.501		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2626.00		NIST Webbook
rinpol	2626.00		NIST Webbook
tb	912.78	K	Joback Method
tc	1137.28	K	Joback Method
tf	543.34	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.23	J/mol×K	912.78	Joback Method
cpg	880.84	J/mol×K	950.20	Joback Method
cpg	893.01	J/mol×K	987.61	Joback Method
cpg	903.76	J/mol×K	1025.03	Joback Method
cpg	913.13	J/mol×K	1062.45	Joback Method
cpg	921.14	J/mol×K	1099.87	Joback Method
cpg	927.82	J/mol×K	1137.28	Joback Method
dvisc	0.0003621	Pa×s	543.34	Joback Method

dvisc	0.0001988	Pa×s	604.91	Joback Method
dvisc	0.0001220	Pa×s	666.49	Joback Method
dvisc	0.0000813	Pa×s	728.06	Joback Method
dvisc	0.0000577	Pa×s	789.63	Joback Method
dvisc	0.0000430	Pa×s	851.21	Joback Method
dvisc	0.0000334	Pa×s	912.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349592&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

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