Succinic acid, 2-methylpent-3-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H28O5/c1-4-21(17(2)3)28-23(25)14-13-22(24)26-16-18-9-8-12-20(15-18)2

InchiKey: FNBJASYFJHMCLK-UHFFFAOYSA-N

Formula: C23H28O5

SMILES: CCC(OC(=O)CCC(=O)OCc1cccc(Oc2ccccc2)c1)C(C)C

Mol. weight [g/mol]: 384.47

Physical Properties

Property code	Value	Unit	Source
gf	-219.75	kJ/mol	Joback Method
hf	-688.84	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	91.95	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.280		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2734.00		NIST Webbook
rinpol	2734.00		NIST Webbook
tb	958.10	K	Joback Method
tc	1184.39	K	Joback Method
tf	550.88	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.42	J/mol×K	958.10	Joback Method
cpg	1038.31	J/mol×K	1146.68	Joback Method
cpg	1030.70	J/mol×K	1108.96	Joback Method
cpg	1021.63	J/mol×K	1071.25	Joback Method
cpg	1011.09	J/mol×K	1033.53	Joback Method
cpg	999.03	J/mol×K	995.82	Joback Method
cpg	1044.51	J/mol×K	1184.39	Joback Method
dvisc	0.0000227	Pa×s	958.10	Joback Method

dvisc	0.0000298	Pa×s	890.23	Joback Method
dvisc	0.0000410	Pa×s	822.36	Joback Method
dvisc	0.0000596	Pa×s	754.49	Joback Method
dvisc	0.0000933	Pa×s	686.62	Joback Method
dvisc	0.0001613	Pa×s	618.75	Joback Method
dvisc	0.0003191	Pa×s	550.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390366&Units=SI

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