

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

Inchi:	InChI=1S/C22H26O5/c1-16(2)17(3)26-22(24)13-12-21(23)25-15-18-8-7-11-20(14-18)27-
InchiKey:	BKXKJDNQIDXKHE-UHFFFAOYSA-N
Formula:	C22H26O5
SMILES:	CC(C)C(C)OC(=O)CCC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	370.44

Physical Properties

Property code	Value	Unit	Source
gf	-228.17	kJ/mol	Joback Method
hf	-668.20	kJ/mol	Joback Method
hfus	40.15	kJ/mol	Joback Method
hvap	89.73	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.890		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinsol	2656.00		NIST Webbook
tb	935.22	K	Joback Method
tc	1161.43	K	Joback Method
tf	539.61	K	Joback Method
vc	1.105	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.30	J/molxK	935.22	Joback Method
cpg	939.97	J/molxK	972.92	Joback Method
cpg	952.13	J/molxK	1010.62	Joback Method
cpg	962.80	J/molxK	1048.33	Joback Method
cpg	972.02	J/molxK	1086.03	Joback Method
cpg	979.81	J/molxK	1123.73	Joback Method
cpg	986.21	J/molxK	1161.43	Joback Method
dvisc	0.0003588	Paxs	539.61	Joback Method
dvisc	0.0001832	Paxs	605.55	Joback Method

dvisc	0.0001067	Paxs	671.48	Joback Method
dvisc	0.0000685	Paxs	737.41	Joback Method
dvisc	0.0000473	Paxs	803.35	Joback Method
dvisc	0.0000345	Paxs	869.29	Joback Method
dvisc	0.0000263	Paxs	935.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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