Succinic acid, 3-methylbut-2-en-1-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C22H24O5/c1-17(2)13-14-25-21(23)11-12-22(24)26-16-18-7-6-10-20(15-18)27

InchiKey: AQHZRQQUNYLAGC-UHFFFAOYSA-N

Formula: C22H24O5

SMILES: CC(C)=CCOC(=O)CCC(=O)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 368.42

Physical Properties

Property code	Value	Unit	Source
gf	-151.62	kJ/mol	Joback Method
hf	-550.21	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.812		Crippen Method
mcvol	289.770	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2763.00		NIST Webbook
tb	940.14	K	Joback Method
tc	1168.62	K	Joback Method
tf	550.57	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.53	J/mol×K	940.14	Joback Method
cpg	909.89	J/mol×K	978.22	Joback Method
cpg	921.91	J/mol×K	1016.30	Joback Method
cpg	932.63	J/mol×K	1054.38	Joback Method
cpg	942.10	J/mol×K	1092.46	Joback Method
cpg	950.37	J/mol×K	1130.54	Joback Method
cpg	957.48	J/mol×K	1168.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390367&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
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