

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

Inchi:	InChI=1S/C22H24O4/c1-17(2)15-16-25-20(23)13-14-21(24)26-22(18-9-5-3-6-10-18)19-1
InchiKey:	JFBOPEBRHOWERJ-UHFFFAOYSA-N
Formula:	C22H24O4
SMILES:	CC(C)=CCOC(=O)CCC(=O)OC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	352.42

Physical Properties

Property code	Value	Unit	Source
gf	-39.43	kJ/mol	Joback Method
hf	-411.80	kJ/mol	Joback Method
hfus	41.76	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.609		Crippen Method
mvol	283.900	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2628.00		NIST Webbook
tb	912.30	K	Joback Method
tc	1142.94	K	Joback Method
tf	500.82	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.02	J/mol×K	912.30	Joback Method
cpg	885.41	J/mol×K	950.74	Joback Method
cpg	898.53	J/mol×K	989.18	Joback Method
cpg	910.45	J/mol×K	1027.62	Joback Method
cpg	921.25	J/mol×K	1066.06	Joback Method
cpg	931.01	J/mol×K	1104.50	Joback Method
cpg	939.80	J/mol×K	1142.94	Joback Method

Sources

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=U390167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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