

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

Inchi: InChI=1S/C23H28O4/c1-4-20(17(2)3)26-21(24)15-16-22(25)27-23(18-11-7-5-8-12-18)19
InchiKey: UTZSTEMVTBWDJG-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: CCC(OC(=O)CCC(=O)OC(c1ccccc1)c1ccccc1)C(C)C
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-107.56	kJ/mol	Joback Method
hf	-550.43	kJ/mol	Joback Method
hfus	38.41	kJ/mol	Joback Method
hvap	88.49	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.077		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	930.26	K	Joback Method
tc	1157.35	K	Joback Method
tf	501.13	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.43	J/molxK	930.26	Joback Method
cpg	974.20	J/molxK	968.11	Joback Method
cpg	987.53	J/molxK	1005.96	Joback Method
cpg	999.47	J/molxK	1043.80	Joback Method
cpg	1010.08	J/molxK	1081.65	Joback Method
cpg	1019.43	J/molxK	1119.50	Joback Method
cpg	1027.57	J/molxK	1157.35	Joback Method
dvisc	0.0006217	Paxs	501.13	Joback Method

dvisc	0.0002669	Paxs	572.65	Joback Method
dvisc	0.0001382	Paxs	644.17	Joback Method
dvisc	0.0000817	Paxs	715.70	Joback Method
dvisc	0.0000531	Paxs	787.22	Joback Method
dvisc	0.0000371	Paxs	858.74	Joback Method
dvisc	0.0000274	Paxs	930.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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