

Succinic acid, dec-2-yl 3-phenylpropyl ester

Inchi:	InChI=1S/C23H36O4/c1-3-4-5-6-7-9-13-20(2)27-23(25)18-17-22(24)26-19-12-16-21-14-
InchiKey:	ANPANTBTWVZTOY-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCCCCCC(C)OC(=O)CCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]:	376.53

Physical Properties

Property code	Value	Unit	Source
gf	-215.09	kJ/mol	Joback Method
hf	-776.40	kJ/mol	Joback Method
hfus	51.42	kJ/mol	Joback Method
hvap	86.99	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.625		Crippen Method
mvol	326.050	ml/mol	McGowan Method
pc	1114.82	kPa	Joback Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook
tb	904.46	K	Joback Method
tc	1110.21	K	Joback Method
tf	504.71	K	Joback Method
vc	1.258	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.07	J/molxK	904.46	Joback Method
cpg	1075.98	J/molxK	938.75	Joback Method
cpg	1091.59	J/molxK	973.04	Joback Method
cpg	1105.94	J/molxK	1007.34	Joback Method
cpg	1119.07	J/molxK	1041.63	Joback Method
cpg	1131.01	J/molxK	1075.92	Joback Method
cpg	1141.81	J/molxK	1110.21	Joback Method
dvisc	0.0005680	Paxs	504.71	Joback Method

dvisc	0.0002660	Paxs	571.33	Joback Method
dvisc	0.0001459	Paxs	637.96	Joback Method
dvisc	0.0000897	Paxs	704.58	Joback Method
dvisc	0.0000600	Paxs	771.21	Joback Method
dvisc	0.0000427	Paxs	837.83	Joback Method
dvisc	0.0000320	Paxs	904.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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