Succinic acid, dodec-2-en-1-yl 2-methoxyphenyl ester

Inchi: InChI=1S/C23H34O5/c1-3-4-5-6-7-8-9-10-11-14-19-27-22(24)17-18-23(25)28-21-16-13-1

InchiKey: MUBZVTPSYBOHEO-SDNWHVSQSA-N

Formula: C23H34O5

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)Oc1ccccc1OC

Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-247.06	kJ/mol	Joback Method
hf	-797.59	kJ/mol	Joback Method
hfus	55.94	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.621		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	2901.00		NIST Webbook
rinpol	2901.00		NIST Webbook
tb	936.46	K	Joback Method
tc	1148.00	K	Joback Method
tf	549.38	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.82	J/mol×K	936.46	Joback Method
cpg	1075.61	J/mol×K	971.72	Joback Method
cpg	1090.07	J/mol×K	1006.97	Joback Method
cpg	1103.24	J/mol×K	1042.23	Joback Method
cpg	1115.16	J/mol×K	1077.49	Joback Method
cpg	1125.86	J/mol×K	1112.74	Joback Method
cpg	1135.37	J/mol×K	1148.00	Joback Method
dvisc	0.0002765	Pa×s	549.38	Joback Method

dvisc	0.0001473	Pa×s	613.89	Joback Method
dvisc	0.0000884	Pa×s	678.41	Joback Method
dvisc	0.0000580	Pa×s	742.92	Joback Method
dvisc	0.0000407	Pa×s	807.43	Joback Method
dvisc	0.0000301	Pa×s	871.95	Joback Method
dvisc	0.0000232	Pa×s	936.46	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=U389719&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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