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

Inchi: InChI=1S/C27H36O4/c1-2-3-4-5-6-7-8-9-10-13-20-30-26(28)18-19-27(29)31-22-23-16-17

InchiKey: BRPKKROVUKGCRJ-JLHYYAGUSA-N

Formula: C27H36O4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-1.73	kJ/mol	Joback Method
hf	-556.86	kJ/mol	Joback Method
hfus	62.13	kJ/mol	Joback Method
hvap	98.54	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	6.903		Crippen Method
mcvol	358.650	ml/mol	McGowan Method
pc	1037.23	kPa	Joback Method
rinpol	3421.00		NIST Webbook
rinpol	3421.00		NIST Webbook
tb	1024.54	K	Joback Method
tc	1254.38	K	Joback Method
tf	604.93	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.38	J/mol×K	1024.54	Joback Method
cpg	1211.55	J/mol×K	1062.85	Joback Method
cpg	1226.62	J/mol×K	1101.15	Joback Method
cpg	1240.68	J/mol×K	1139.46	Joback Method
cpg	1253.85	J/mol×K	1177.77	Joback Method
cpg	1266.22	J/mol×K	1216.07	Joback Method
cpg	1277.91	J/mol×K	1254.38	Joback Method
dvisc	0.0003291	Pa×s	604.93	Joback Method

dvisc	0.0001886	Pa×s	674.87	Joback Method
dvisc	0.0001200	Pa×s	744.80	Joback Method
dvisc	0.0000825	Pa×s	814.74	Joback Method
dvisc	0.0000602	Pa×s	884.67	Joback Method
dvisc	0.0000460	Pa×s	954.61	Joback Method
dvisc	0.0000364	Pa×s	1024.54	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390011&Units=SI

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