Succinic acid, naphth-2-ylmethyl trans-hex-3-en-1-yl ester

Inchi: InChI=1S/C21H24O4/c1-2-3-4-7-14-24-20(22)12-13-21(23)25-16-17-10-11-18-8-5-6-9-19

InchiKey: OFNOTDCPCMXRGU-ONEGZZNKSA-N

Formula: C21H24O4

SMILES: CCC=CCCOC(=O)CCC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-52.25	kJ/mol	Joback Method
hf	-433.02	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	85.19	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.563		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	2819.00		NIST Webbook
rinpol	2819.00		NIST Webbook
tb	887.26	K	Joback Method
tc	1105.52	K	Joback Method
tf	537.31	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.53	J/mol×K	887.26	Joback Method
cpg	847.89	J/mol×K	923.64	Joback Method
cpg	861.24	J/mol×K	960.01	Joback Method
cpg	873.66	J/mol×K	996.39	Joback Method
cpg	885.22	J/mol×K	1032.77	Joback Method
cpg	895.98	J/mol×K	1069.14	Joback Method
cpg	906.02	J/mol×K	1105.52	Joback Method
dvisc	0.0005983	Pa×s	537.31	Joback Method

dvisc	0.0003668	Pa×s	595.63	Joback Method
dvisc	0.0002454	Pa×s	653.96	Joback Method
dvisc	0.0001753	Pa×s	712.28	Joback Method
dvisc	0.0001318	Pa×s	770.61	Joback Method
dvisc	0.0001031	Pa×s	828.93	Joback Method
dvisc	0.0000834	Pa×s	887.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391127&Units=SI
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

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