Succinic acid, naphth-2-ylmethyl cis-4-methylcyclohexyl ester

Inchi: InChI=1S/C22H26O4/c1-16-6-10-20(11-7-16)26-22(24)13-12-21(23)25-15-17-8-9-18-4-2

InchiKey: JGSCGESOTFPLKS-MOBUCQHHSA-N

Formula: C22H26O4

SMILES: C[C@H]1CC[C@@H](OC(=O)CCC(=O)OCc2ccc3ccccc3c2)CC1

Mol. weight [g/mol]: 354.45

Physical Properties

Property code	Value	Unit	Source
hfus	45.05	kJ/mol	Joback Method
logp	4.785		Crippen Method
mcvol	281.640	ml/mol	McGowan Method
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-7.70070e+01
Coeff. B	1.93772e+00
Coeff. C	-1.11028e-03
Coeff. D	1.99500e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s

Coeff. A	-1.24474e+01
Coeff. B	2.72258e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	497.14
Temperature range (K), max.	780.09

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U390064&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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