Succinic acid, naphth-2-ylmethyl 3-heptyl ester

Inchi: InChI=1S/C22H28O4/c1-3-5-10-20(4-2)26-22(24)14-13-21(23)25-16-17-11-12-18-8-6-7-9

InchiKey: YOHQMGSAYDOZQV-UHFFFAOYSA-N

Formula: C22H28O4

SMILES: CCCCC(CC)OC(=O)CCC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 356.46

Physical Properties

Property code	Value	Unit	Source
gf	-126.49	kJ/mol	Joback Method
hf	-576.16	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	87.07	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.175		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		NIST Webbook
tb	905.54	K	Joback Method
tc	1121.21	K	Joback Method
tf	538.66	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.50	J/mol×K	905.54	Joback Method
cpg	935.52	J/mol×K	941.48	Joback Method
cpg	949.40	J/mol×K	977.43	Joback Method
cpg	962.20	J/mol×K	1013.37	Joback Method
cpg	973.97	J/mol×K	1049.32	Joback Method
cpg	984.77	J/mol×K	1085.26	Joback Method
cpg	994.66	J/mol×K	1121.21	Joback Method
dvisc	0.0006454	Pa×s	538.66	Joback Method

dvisc	0.0003770	Pa×s	599.81	Joback Method
dvisc	0.0002432	Pa×s	660.95	Joback Method
dvisc	0.0001690	Pa×s	722.10	Joback Method
dvisc	0.0001243	Pa×s	783.25	Joback Method
dvisc	0.0000956	Pa×s	844.39	Joback Method
dvisc	0.0000762	Pa×s	905.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390613&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

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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