Succinic acid, cis-hex-3-enyl propyl ester

Inchi: InChI=1S/C13H22O4/c1-3-5-6-7-11-17-13(15)9-8-12(14)16-10-4-2/h5-6H,3-4,7-11H2,1-2
InchiKey: LDLIWNHOZGTWJR-WAYWQWQTSA-N
Formula: C13H22O4
SMILES: CCC=CCCOC(=O)CCC(=O)OCCC
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-329.04	kJ/mol	Joback Method
hf	-684.03	kJ/mol	Joback Method
hfus	35.20	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.619		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
tb	653.58	K	Joback Method
tc	835.79	K	Joback Method
tf	375.51	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.88	J/mol×K	653.58	Joback Method
cpg	613.22	J/mol×K	805.43	Joback Method
cpg	601.30	J/mol×K	775.06	Joback Method
cpg	588.72	J/mol×K	744.69	Joback Method
cpg	575.46	J/mol×K	714.32	Joback Method
cpg	561.52	J/mol×K	683.95	Joback Method
cpg	624.48	J/mol×K	835.79	Joback Method
dvisc	0.0001162	Pa×s	653.58	Joback Method

dvisc	0.0001511	Pa×s	607.23	Joback Method
dvisc	0.0002051	Pa×s	560.89	Joback Method
dvisc	0.0002942	Pa×s	514.54	Joback Method
dvisc	0.0004533	Pa×s	468.20	Joback Method
dvisc	0.0007681	Pa×s	421.85	Joback Method
dvisc	0.0014825	Pa×s	375.51	Joback Method

Sources

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=U353404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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