Succinic acid, cyclohexylmethyl hex-5-en-1-yl ester

Inchi: InChI=1S/C17H28O4/c1-2-3-4-8-13-20-16(18)11-12-17(19)21-14-15-9-6-5-7-10-15/h2,15

InchiKey: JZMGDRAMNCYXIB-UHFFFAOYSA-N

Formula: C17H28O4

SMILES: C=CCCCCOC(=O)CCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-263.29	kJ/mol	Joback Method
hf	-704.06	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	71.51	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.790		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	757.17	K	Joback Method
tc	954.78	K	Joback Method
tf	431.29	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.31	J/mol×K	757.17	Joback Method
cpg	779.34	J/mol×K	790.11	Joback Method
cpg	796.22	J/mol×K	823.04	Joback Method
cpg	811.96	J/mol×K	855.98	Joback Method
cpg	826.59	J/mol×K	888.91	Joback Method
cpg	840.13	J/mol×K	921.85	Joback Method
cpg	852.59	J/mol×K	954.78	Joback Method
dvisc	0.0013346	Pa×s	431.29	Joback Method

dvisc	0.0006614	Pa×s	485.60	Joback Method
dvisc	0.0003775	Pa×s	539.92	Joback Method
dvisc	0.0002388	Pa×s	594.23	Joback Method
dvisc	0.0001630	Pa×s	648.54	Joback Method
dvisc	0.0001181	Pa×s	702.86	Joback Method
dvisc	0.0000896	Pa×s	757.17	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=U391285&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