Succinic acid, cyclohexylmethyl dec-9-en-1-yl ester

Inchi: InChI=1S/C21H36O4/c1-2-3-4-5-6-7-8-12-17-24-20(22)15-16-21(23)25-18-19-13-10-9-11

InchiKey: SAXISOJTVYWCGG-UHFFFAOYSA-N

Formula: C21H36O4

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

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-229.61	kJ/mol	Joback Method
hf	-786.62	kJ/mol	Joback Method
hfus	46.27	kJ/mol	Joback Method
hvap	80.41	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.350		Crippen Method
mcvol	306.470	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	848.69	K	Joback Method
tc	1046.95	K	Joback Method
tf	476.37	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.81	J/mol×K	848.69	Joback Method
cpg	1079.89	J/mol×K	1013.91	Joback Method
cpg	1066.36	J/mol×K	980.87	Joback Method
cpg	1051.62	J/mol×K	947.82	Joback Method
cpg	1035.64	J/mol×K	914.78	Joback Method
cpg	1018.37	J/mol×K	881.73	Joback Method
cpg	1092.22	J/mol×K	1046.95	Joback Method
dvisc	0.0000509	Pa×s	848.69	Joback Method

dvisc	0.0000679	Pa×s	786.64	Joback Method
dvisc	0.0000949	Pa×s	724.58	Joback Method
dvisc	0.0001414	Pa×s	662.53	Joback Method
dvisc	0.0002288	Pa×s	600.48	Joback Method
dvisc	0.0004134	Pa×s	538.42	Joback Method
dvisc	0.0008717	Pa×s	476.37	Joback Method

Sources

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=U391251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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