Succinic acid, cyclohexylmethyl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi: InChI=1S/C19H30O4/c1-15-7-5-6-10-17(15)14-23-19(21)12-11-18(20)22-13-16-8-3-2-4-9

InchiKey: NJJFXGNPGTUADD-UHFFFAOYSA-N

Formula: C19H30O4

SMILES: CC1=C(COC(=O)CCC(=O)OCC2CCCCC2)CCCC1

Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-291.43	kJ/mol	Joback Method
hf	-761.27	kJ/mol	Joback Method
hfus	33.58	kJ/mol	Joback Method
hvap	78.98	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.324		Crippen Method
mcvol	267.430	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	839.59	K	Joback Method
tc	1057.98	K	Joback Method
tf	493.01	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.39	J/mol×K	839.59	Joback Method
cpg	888.96	J/mol×K	875.99	Joback Method
cpg	905.97	J/mol×K	912.39	Joback Method
cpg	921.46	J/mol×K	948.78	Joback Method
cpg	935.44	J/mol×K	985.18	Joback Method
cpg	947.94	J/mol×K	1021.58	Joback Method
cpg	958.99	J/mol×K	1057.98	Joback Method
dvisc	0.0007746	Pa×s	493.01	Joback Method

dvisc	0.0003977	Pa×s	550.77	Joback Method
dvisc	0.0002317	Pa×s	608.54	Joback Method
dvisc	0.0001483	Pa×s	666.30	Joback Method
dvisc	0.0001019	Pa×s	724.06	Joback Method
dvisc	0.0000740	Pa×s	781.83	Joback Method
dvisc	0.0000562	Pa×s	839.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391420&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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