Succinic acid, hept-2-yl (2-chlorocyclohexyl)methyl ester

Inchi: InChI=1S/C18H31ClO4/c1-3-4-5-8-14(2)23-18(21)12-11-17(20)22-13-15-9-6-7-10-16(15)

InchiKey: YTQIMVBLULCHJJ-UHFFFAOYSA-N

Formula: C18H31ClO4

SMILES: CCCCCC(C)OC(=O)CCC(=O)OCC1CCCCC1Cl

Mol. weight [g/mol]: 346.89

Physical Properties

Property code	Value	Unit	Source
gf	-364.79	kJ/mol	Joback Method
hf	-891.49	kJ/mol	Joback Method
hfus	41.53	kJ/mol	Joback Method
hvap	78.09	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.619		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	815.69	K	Joback Method
tc	1016.89	K	Joback Method
tf	455.00	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.88	J/mol×K	815.69	Joback Method
cpg	957.65	J/mol×K	983.36	Joback Method
cpg	944.84	J/mol×K	949.82	Joback Method
cpg	930.78	J/mol×K	916.29	Joback Method
cpg	915.44	J/mol×K	882.76	Joback Method
cpg	898.81	J/mol×K	849.22	Joback Method
cpg	969.22	J/mol×K	1016.89	Joback Method
dvisc	0.0000744	Pa×s	815.69	Joback Method

dvisc	0.0000980	Pa×s	755.57	Joback Method
dvisc	0.0001354	Pa×s	695.46	Joback Method
dvisc	0.0001989	Pa×s	635.35	Joback Method
dvisc	0.0003168	Pa×s	575.23	Joback Method
dvisc	0.0005622	Pa×s	515.12	Joback Method
dvisc	0.0011610	Pa×s	455.00	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=U391400&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