Succinic acid, 2,2-dichloroethyl cis-hex-2-en-1-yl ester

Inchi: InChI=1S/C12H18Cl2O4/c1-2-3-4-5-8-17-11(15)6-7-12(16)18-9-10(13)14/h4-5,10H,2-3,6

InchiKey: ORLYGSSKIUQJBX-PLNGDYQASA-N

Formula: C12H18Cl2O4

SMILES: CCCC=CCOC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 297.18

Physical Properties

Property code	Value	Unit	Source
gf	-363.76	kJ/mol	Joback Method
hf	-700.15	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	68.96	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.013		Crippen Method
mcvol	215.000	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	705.12	K	Joback Method
tc	899.84	K	Joback Method
tf	409.08	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.21	J/mol×K	705.12	Joback Method
cpg	606.49	J/mol×K	867.38	Joback Method
cpg	596.63	J/mol×K	834.93	Joback Method
cpg	586.09	J/mol×K	802.48	Joback Method
cpg	574.84	J/mol×K	770.03	Joback Method
cpg	562.89	J/mol×K	737.57	Joback Method
cpg	615.68	J/mol×K	899.84	Joback Method
dvisc	0.0000986	Pa×s	705.12	Joback Method

dvisc	0.0001292	Pa×s	655.78	Joback Method
dvisc	0.0001769	Pa×s	606.44	Joback Method
dvisc	0.0002561	Pa×s	557.10	Joback Method
dvisc	0.0003985	Pa×s	507.76	Joback Method
dvisc	0.0006818	Pa×s	458.42	Joback Method
dvisc	0.0013278	Pa×s	409.08	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=U391300&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