Succinic acid, 2,2-dichloroethyl hex-5-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/h2,10H,1,3-9H

InchiKey: XTVYLAJSHRJWKH-UHFFFAOYSA-N

Formula: C12H18Cl2O4

SMILES: C=CCCCCOC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 297.18

Physical Properties

Property code	Value	Unit	Source
gf	-356.14	kJ/mol	Joback Method
hf	-691.94	kJ/mol	Joback Method
hfus	36.00	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.013		Crippen Method
mcvol	215.000	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
tb	697.64	K	Joback Method
tc	888.98	K	Joback Method
tf	412.40	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.91	J/mol×K	697.64	Joback Method
cpg	562.57	J/mol×K	729.53	Joback Method
cpg	574.53	J/mol×K	761.42	Joback Method
cpg	585.77	J/mol×K	793.31	Joback Method
cpg	596.32	J/mol×K	825.20	Joback Method
cpg	606.17	J/mol×K	857.09	Joback Method
cpg	615.34	J/mol×K	888.98	Joback Method
dvisc	0.0014280	Pa×s	412.40	Joback Method

dvisc	0.0007646	Pa×s	459.94	Joback Method
dvisc	0.0004603	Pa×s	507.48	Joback Method
dvisc	0.0003022	Pa×s	555.02	Joback Method
dvisc	0.0002121	Pa×s	602.56	Joback Method
dvisc	0.0001567	Pa×s	650.10	Joback Method
dvisc	0.0001207	Pa×s	697.64	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=U391282&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