Succinic acid, 2-chlorophenyl 2-chloroethyl ester

Inchi: InChI=1S/C12H12Cl2O4/c13-7-8-17-11(15)5-6-12(16)18-10-4-2-1-3-9(10)14/h1-4H,5-8H

InchiKey: HMFXHQHRCNNEOF-UHFFFAOYSA-N

Formula: C12H12Cl2O4

SMILES: O=C(CCC(=O)Oc1ccccc1Cl)OCCCl

Mol. weight [g/mol]: 291.13

Physical Properties

Property code	Value	Unit	Source
gf	-338.76	kJ/mol	Joback Method
hf	-587.03	kJ/mol	Joback Method
hfus	34.46	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.808		Crippen Method
mcvol	195.540	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	2112.00		NIST Webbook
tb	733.06	K	Joback Method
tc	951.25	K	Joback Method
tf	468.10	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.74	J/mol×K	733.06	Joback Method
cpg	496.09	J/mol×K	769.43	Joback Method
cpg	506.58	J/mol×K	805.79	Joback Method
cpg	516.22	J/mol×K	842.16	Joback Method
cpg	525.03	J/mol×K	878.52	Joback Method
cpg	533.00	J/mol×K	914.89	Joback Method
cpg	540.14	J/mol×K	951.25	Joback Method
dvisc	0.0008555	Pa×s	468.10	Joback Method
dvisc	0.0005397	Pa×s	512.26	Joback Method

dvisc	0.0003663	Pa×s	556.42	Joback Method
dvisc	0.0002632	Pa×s	600.58	Joback Method
dvisc	0.0001978	Pa×s	644.74	Joback Method
dvisc	0.0001543	Pa×s	688.90	Joback Method
dvisc	0.0001240	Pa×s	733.06	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=U357547&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