Succinic acid, phenyl 2-chloroethyl ester

Inchi: InChI=1S/C12H13ClO4/c13-8-9-16-11(14)6-7-12(15)17-10-4-2-1-3-5-10/h1-5H,6-9H2
InchiKey: WETSIKFDVBOWKR-UHFFFAOYSA-N
Formula: C12H13ClO4
SMILES: O=C(CCC(=O)Oc1ccccc1)OCCCl
Mol. weight [g/mol]: 256.68

Physical Properties

Property code	Value	Unit	Source
gf	-317.20	kJ/mol	Joback Method
hf	-559.82	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	67.28	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.154		Crippen Method
mcvol	183.300	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1952.00		NIST Webbook
tb	690.65	K	Joback Method
tc	904.92	K	Joback Method
tf	425.66	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.62	J/mol×K	690.65	Joback Method
cpg	475.14	J/mol×K	726.36	Joback Method
cpg	486.79	J/mol×K	762.07	Joback Method
cpg	497.59	J/mol×K	797.79	Joback Method
cpg	507.55	J/mol×K	833.50	Joback Method
cpg	516.68	J/mol×K	869.21	Joback Method
cpg	524.99	J/mol×K	904.92	Joback Method
dvisc	0.0011839	Pa×s	425.66	Joback Method
dvisc	0.0006997	Pa×s	469.82	Joback Method

dvisc	0.0004526	Pa×s	513.99	Joback Method
dvisc	0.0003137	Pa×s	558.15	Joback Method
dvisc	0.0002294	Pa×s	602.32	Joback Method
dvisc	0.0001751	Pa×s	646.48	Joback Method
dvisc	0.0001384	Pa×s	690.65	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=U357987&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