Succinic acid, 2,2-dichloroethyl 4-chlorobenzyl ester

Inchi: InChI=1S/C13H13Cl3O4/c14-10-3-1-9(2-4-10)7-19-12(17)5-6-13(18)20-8-11(15)16/h1-4,

InchiKey: SPVDDTWLOBNMJG-UHFFFAOYSA-N

Formula: C13H13Cl3O4

SMILES: O=C(CCC(=O)OCC(Cl)Cl)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 339.60

Physical Properties

Property code	Value	Unit	Source
gf	-344.71	kJ/mol	Joback Method
hf	-628.69	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.510		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	2338.00		NIST Webbook
rinpol	2338.00		NIST Webbook
tb	792.93	K	Joback Method
tc	1014.67	K	Joback Method
tf	494.29	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.79	J/mol×K	792.93	Joback Method
cpg	570.68	J/mol×K	829.89	Joback Method
cpg	580.63	J/mol×K	866.84	Joback Method
cpg	589.64	J/mol×K	903.80	Joback Method
cpg	597.74	J/mol×K	940.76	Joback Method
cpg	604.93	J/mol×K	977.72	Joback Method
cpg	611.23	J/mol×K	1014.67	Joback Method
dvisc	0.0007418	Pa×s	494.29	Joback Method

dvisc	0.0004414	Pa×s	544.06	Joback Method
dvisc	0.0002865	Pa×s	593.84	Joback Method
dvisc	0.0001988	Pa×s	643.61	Joback Method
dvisc	0.0001454	Pa×s	693.38	Joback Method
dvisc	0.0001109	Pa×s	743.16	Joback Method
dvisc	0.0000875	Pa×s	792.93	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=U389673&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