Succinic acid, 2,2-dichloroethyl 2-chloro-4-methylphenyl ester

Inchi: InChI=1S/C13H13Cl3O4/c1-8-2-3-10(9(14)6-8)20-13(18)5-4-12(17)19-7-11(15)16/h2-3,6

InchiKey: XBPMFLPDFBJDFP-UHFFFAOYSA-N

Formula: C13H13Cl3O4

SMILES: Cc1ccc(OC(=O)CCC(=O)OCC(Cl)Cl)c(Cl)c1

Mol. weight [g/mol]: 339.60

Physical Properties

Property code	Value	Unit	Source
gf	-354.34	kJ/mol	Joback Method
hf	-640.16	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.681		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2312.00		NIST Webbook
rinpol	2312.00		NIST Webbook
tb	797.91	K	Joback Method
tc	1020.41	K	Joback Method
tf	506.81	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.19	J/mol×K	797.91	Joback Method
cpg	602.90	J/mol×K	983.33	Joback Method
cpg	595.81	J/mol×K	946.24	Joback Method
cpg	587.80	J/mol×K	909.16	Joback Method
cpg	578.86	J/mol×K	872.08	Joback Method
cpg	568.99	J/mol×K	834.99	Joback Method
cpg	609.08	J/mol×K	1020.41	Joback Method
dvisc	0.0000882	Pa×s	797.91	Joback Method

dvisc	0.0001103	Pa×s	749.39	Joback Method
dvisc	0.0001422	Pa×s	700.88	Joback Method
dvisc	0.0001905	Pa×s	652.36	Joback Method
dvisc	0.0002674	Pa×s	603.84	Joback Method
dvisc	0.0003983	Pa×s	555.33	Joback Method
dvisc	0.0006402	Pa×s	506.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U390215&Units=SI

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