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

Inchi: InChI=1S/C13H13Cl3O5/c1-19-10-6-8(14)2-3-9(10)21-13(18)5-4-12(17)20-7-11(15)16/h2

InchiKey: ZIKJQFZTRXMLAA-UHFFFAOYSA-N

Formula: C13H13Cl3O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 355.60

Physical Properties

Property code	Value	Unit	Source
gf	-459.34	kJ/mol	Joback Method
hf	-772.38	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	81.62	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.381		Crippen Method
mcvol	227.740	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	820.33	K	Joback Method
tc	1041.11	K	Joback Method
tf	529.04	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.93	J/mol×K	820.33	Joback Method
cpg	593.36	J/mol×K	857.13	Joback Method
cpg	602.80	J/mol×K	893.92	Joback Method
cpg	611.22	J/mol×K	930.72	Joback Method
cpg	618.62	J/mol×K	967.51	Joback Method
cpg	624.99	J/mol×K	1004.31	Joback Method
cpg	630.31	J/mol×K	1041.11	Joback Method
dvisc	0.0004568	Pa×s	529.04	Joback Method

dvisc	0.0002893	Pa×s	577.59	Joback Method
dvisc	0.0001966	Pa×s	626.14	Joback Method
dvisc	0.0001413	Pa×s	674.68	Joback Method
dvisc	0.0001061	Pa×s	723.23	Joback Method
dvisc	0.0000826	Pa×s	771.78	Joback Method
dvisc	0.0000663	Pa×s	820.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390935&Units=SI
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

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