Succinic acid, 2,4,6-trichlorophenyl 2-methoxyethyl ester

Inchi: InChI=1S/C13H13Cl3O5/c1-19-4-5-20-11(17)2-3-12(18)21-13-9(15)6-8(14)7-10(13)16/h6

InchiKey: UOXUVKZZXJWCPX-UHFFFAOYSA-N

Formula: C13H13Cl3O5

SMILES: COCCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 355.60

Physical Properties

Property code	Value	Unit	Source
gf	-466.53	kJ/mol	Joback Method
hf	-778.57	kJ/mol	Joback Method
hfus	41.65	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.522		Crippen Method
mcvol	227.740	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	825.75	K	Joback Method
tc	1044.21	K	Joback Method
tf	556.56	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.66	J/mol×K	825.75	Joback Method
cpg	590.88	J/mol×K	862.16	Joback Method
cpg	600.14	J/mol×K	898.57	Joback Method
cpg	608.42	J/mol×K	934.98	Joback Method
cpg	615.70	J/mol×K	971.39	Joback Method
cpg	621.97	J/mol×K	1007.80	Joback Method
cpg	627.21	J/mol×K	1044.21	Joback Method
dvisc	0.0003737	Pa×s	556.56	Joback Method

dvisc	0.0002572	Pa×s	601.43	Joback Method
dvisc	0.0001865	Pa×s	646.29	Joback Method
dvisc	0.0001409	Pa×s	691.15	Joback Method
dvisc	0.0001102	Pa×s	736.02	Joback Method
dvisc	0.0000887	Pa×s	780.88	Joback Method
dvisc	0.0000731	Pa×s	825.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390749&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