Succinic acid, 2-methylpent-3-yl 2,2-dichloroethyl ester

Inchi: InChI=1S/C12H20Cl2O4/c1-4-9(8(2)3)18-12(16)6-5-11(15)17-7-10(13)14/h8-10H,4-7H2,

InchiKey: XVSKGIPZYKHZDF-UHFFFAOYSA-N

Formula: C12H20Cl2O4

SMILES: CCC(OC(=O)CCC(=O)OCC(Cl)Cl)C(C)C

Mol. weight [g/mol]: 299.19

Physical Properties

Property code	Value	Unit	Source
gf	-448.86	kJ/mol	Joback Method
hf	-827.93	kJ/mol	Joback Method
hfus	30.24	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.091		Crippen Method
mcvol	219.300	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1766.00		NIST Webbook
rinpol	1766.00		NIST Webbook
tb	700.08	K	Joback Method
tc	894.49	K	Joback Method
tf	384.16	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.60	J/mol×K	700.08	Joback Method
cpg	588.30	J/mol×K	732.48	Joback Method
cpg	601.20	J/mol×K	764.88	Joback Method
cpg	613.32	J/mol×K	797.29	Joback Method
cpg	624.66	J/mol×K	829.69	Joback Method
cpg	635.22	J/mol×K	862.09	Joback Method
cpg	645.02	J/mol×K	894.49	Joback Method
dvisc	0.0021572	Pa×s	384.16	Joback Method

dvisc	0.0009443	Pa×s	436.81	Joback Method
dvisc	0.0004937	Pa×s	489.47	Joback Method
dvisc	0.0002928	Pa×s	542.12	Joback Method
dvisc	0.0001905	Pa×s	594.77	Joback Method
dvisc	0.0001329	Pa×s	647.43	Joback Method
dvisc	0.0000979	Pa×s	700.08	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=U390517&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