Succinic acid, 8-chlorooctyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C14H22Cl4O4/c15-9-5-3-1-2-4-6-10-21-12(19)7-8-13(20)22-11-14(16,17)18/h1

InchiKey: MMNQAIFULDGHJQ-UHFFFAOYSA-N

Formula: C14H22Cl4O4

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

Mol. weight [g/mol]: 396.13

Physical Properties

Property code	Value	Unit	Source
gf	-445.72	kJ/mol	Joback Method
hf	-893.60	kJ/mol	Joback Method
hfus	46.96	kJ/mol	Joback Method
hvap	81.31	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.803		Crippen Method
mcvol	271.960	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	818.79	K	Joback Method
tc	1019.31	K	Joback Method
tf	513.96	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.84	J/mol×K	818.79	Joback Method
cpg	747.05	J/mol×K	852.21	Joback Method
cpg	758.41	J/mol×K	885.63	Joback Method
cpg	768.94	J/mol×K	919.05	Joback Method
cpg	778.67	J/mol×K	952.47	Joback Method
cpg	787.63	J/mol×K	985.89	Joback Method
cpg	795.85	J/mol×K	1019.31	Joback Method
dvisc	0.0005950	Pa×s	513.96	Joback Method

dvisc	0.0003345	Pa×s	564.76	Joback Method
dvisc	0.0002068	Pa×s	615.57	Joback Method
dvisc	0.0001376	Pa×s	666.38	Joback Method
dvisc	0.0000969	Pa×s	717.18	Joback Method
dvisc	0.0000716	Pa×s	767.98	Joback Method
dvisc	0.0000549	Pa×s	818.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390243&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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