Sebacic acid, di(2,2,2-trichloroethyl) ester

Inchi: InChI=1S/C14H20Cl6O4/c15-13(16,17)9-23-11(21)7-5-3-1-2-4-6-8-12(22)24-10-14(18,19
InchiKey: XMZNZRMANMWYRT-UHFFFAOYSA-N
Formula: C14H20Cl6O4
SMILES: O=C(CCCCCCCCC(=O)OCC(Cl)(Cl)Cl)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 465.02

Physical Properties

Property code	Value	Unit	Source
gf	-466.74	kJ/mol	Joback Method
hf	-933.83	kJ/mol	Joback Method
hfus	47.94	kJ/mol	Joback Method
hvap	88.79	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.934		Crippen Method
mcvol	296.440	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	890.42	K	Joback Method
tc	1105.77	K	Joback Method
tf	576.22	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.31	J/mol×K	890.42	Joback Method
cpg	790.59	J/mol×K	926.31	Joback Method
cpg	800.05	J/mol×K	962.20	Joback Method
cpg	808.76	J/mol×K	998.09	Joback Method
cpg	816.77	J/mol×K	1033.99	Joback Method
cpg	824.15	J/mol×K	1069.88	Joback Method
cpg	830.96	J/mol×K	1105.77	Joback Method
dvisc	0.0003133	Pa×s	576.22	Joback Method

dvisc	0.0001789	Pa×s	628.59	Joback Method
dvisc	0.0001114	Pa×s	680.95	Joback Method
dvisc	0.0000742	Pa×s	733.32	Joback Method
dvisc	0.0000522	Pa×s	785.69	Joback Method
dvisc	0.0000383	Pa×s	838.05	Joback Method
dvisc	0.0000292	Pa×s	890.42	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=U355321&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