Sebacic acid, 2,2,2-trichloroethyl undecyl ester

Inchi: InChI=1S/C23H41Cl3O4/c1-2-3-4-5-6-7-10-13-16-19-29-21(27)17-14-11-8-9-12-15-18-22

InchiKey: FTTIMINCZKMPGJ-UHFFFAOYSA-N

Formula: C23H41Cl3O4

SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 487.93

Physical Properties

Property code	Value	Unit	Source
gf	-358.01	kJ/mol	Joback Method
hf	-1063.62	kJ/mol	Joback Method
hfus	66.08	kJ/mol	Joback Method
hvap	96.96	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	8.095		Crippen Method
mcvol	386.530	ml/mol	McGowan Method
pc	851.97	kPa	Joback Method
rinpol	3128.00		NIST Webbook
tb	987.28	K	Joback Method
tc	1210.91	K	Joback Method
tf	585.47	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1241.41	J/mol×K	987.28	Joback Method
cpg	1258.03	J/mol×K	1024.55	Joback Method
cpg	1273.31	J/mol×K	1061.82	Joback Method
cpg	1287.33	J/mol×K	1099.09	Joback Method
cpg	1300.14	J/mol×K	1136.36	Joback Method
cpg	1311.84	J/mol×K	1173.63	Joback Method
cpg	1322.48	J/mol×K	1210.91	Joback Method
dvisc	0.0002381	Pa×s	585.47	Joback Method
dvisc	0.0001188	Pa×s	652.44	Joback Method

dvisc	0.0000674	Pa×s	719.41	Joback Method
dvisc	0.0000422	Pa×s	786.38	Joback Method
dvisc	0.0000284	Pa×s	853.34	Joback Method
dvisc	0.0000202	Pa×s	920.31	Joback Method
dvisc	0.0000151	Pa×s	987.28	Joback Method

Sources

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=U355319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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