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

Inchi: InChI=1S/C10H12Cl6O4/c11-9(12,13)5-19-7(17)3-1-2-4-8(18)20-6-10(14,15)16/h1-6H2
InchiKey: ORLGXGVFGFWARG-UHFFFAOYSA-N
Formula: C10H12Cl6O4
SMILES: O=C(CCCCC(=O)OCC(Cl)(Cl)Cl)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 408.92

Physical Properties

Property code	Value	Unit	Source
gf	-500.42	kJ/mol	Joback Method
hf	-851.27	kJ/mol	Joback Method
hfus	37.58	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.374		Crippen Method
mcvol	240.080	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	2858.00		NIST Webbook
tb	798.90	K	Joback Method
tc	1019.94	K	Joback Method
tf	531.14	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.63	J/mol×K	798.90	Joback Method
cpg	573.19	J/mol×K	835.74	Joback Method
cpg	580.99	J/mol×K	872.58	Joback Method
cpg	588.08	J/mol×K	909.42	Joback Method
cpg	594.51	J/mol×K	946.26	Joback Method
cpg	600.35	J/mol×K	983.10	Joback Method
cpg	605.63	J/mol×K	1019.94	Joback Method
dvisc	0.0005317	Pa×s	531.14	Joback Method
dvisc	0.0003192	Pa×s	575.77	Joback Method

dvisc	0.0002062	Pa×s	620.39	Joback Method
dvisc	0.0001412	Pa×s	665.02	Joback Method
dvisc	0.0001015	Pa×s	709.65	Joback Method
dvisc	0.0000758	Pa×s	754.27	Joback Method
dvisc	0.0000585	Pa×s	798.90	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=U353485&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