Adipic acid, propyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C11H17Cl3O4/c1-2-7-17-9(15)5-3-4-6-10(16)18-8-11(12,13)14/h2-8H2,1H3
InchiKey: PBDQYFDNQMMOJM-UHFFFAOYSA-N
Formula: C11H17Cl3O4
SMILES: CCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 319.61

Physical Properties

Property code	Value	Unit	Source
gf	-459.05	kJ/mol	Joback Method
hf	-815.94	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	70.25	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.413		Crippen Method
mcvol	217.450	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1865.00		NIST Webbook
tb	712.72	K	Joback Method
tc	912.17	K	Joback Method
tf	450.23	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.97	J/mol×K	712.72	Joback Method
cpg	560.87	J/mol×K	745.96	Joback Method
cpg	572.01	J/mol×K	779.20	Joback Method
cpg	582.41	J/mol×K	812.44	Joback Method
cpg	592.09	J/mol×K	845.68	Joback Method
cpg	601.07	J/mol×K	878.92	Joback Method
cpg	609.36	J/mol×K	912.17	Joback Method
dvisc	0.0010572	Pa×s	450.23	Joback Method
dvisc	0.0006051	Pa×s	493.98	Joback Method

dvisc	0.0003792	Pa×s	537.73	Joback Method
dvisc	0.0002549	Pa×s	581.48	Joback Method
dvisc	0.0001812	Pa×s	625.22	Joback Method
dvisc	0.0001347	Pa×s	668.97	Joback Method
dvisc	0.0001038	Pa×s	712.72	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=U353474&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