Adipic acid, 2,2,2-trichloroethyl tridecyl ester

Inchi: InChI=1S/C21H37Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-27-19(25)15-12-13-16-20(26)28
InchiKey: SKTHCYOSFPAGPW-UHFFFAOYSA-N
Formula: C21H37Cl3O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 459.88

Physical Properties

Property code	Value	Unit	Source
gf	-374.85	kJ/mol	Joback Method
hf	-1022.34	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.314		Crippen Method
mcvol	358.350	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	941.52	K	Joback Method
tc	1152.69	K	Joback Method
tf	562.93	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.57	J/mol×K	941.52	Joback Method
cpg	1134.30	J/mol×K	976.71	Joback Method
cpg	1148.85	J/mol×K	1011.91	Joback Method
cpg	1162.27	J/mol×K	1047.10	Joback Method
cpg	1174.62	J/mol×K	1082.30	Joback Method
cpg	1185.95	J/mol×K	1117.49	Joback Method
cpg	1196.32	J/mol×K	1152.69	Joback Method
dvisc	0.0003137	Pa×s	562.93	Joback Method

dvisc	0.0001594	Pa×s	626.03	Joback Method
dvisc	0.0000917	Pa×s	689.13	Joback Method
dvisc	0.0000579	Pa×s	752.23	Joback Method
dvisc	0.0000393	Pa×s	815.32	Joback Method
dvisc	0.0000281	Pa×s	878.42	Joback Method
dvisc	0.0000211	Pa×s	941.52	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=U353486&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