Adipic acid, heptyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C15H25Cl3O4/c1-2-3-4-5-8-11-21-13(19)9-6-7-10-14(20)22-12-15(16,17)18/h2
InchiKey: FPEZRQSRNBICGQ-UHFFFAOYSA-N
Formula: C15H25Cl3O4
SMILES: CCCCCCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 375.72

Physical Properties

Property code	Value	Unit	Source
gf	-425.37	kJ/mol	Joback Method
hf	-898.50	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	79.16	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.974		Crippen Method
mcvol	273.810	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	804.24	K	Joback Method
tc	1000.17	K	Joback Method
tf	495.31	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.91	J/mol×K	804.24	Joback Method
cpg	779.48	J/mol×K	836.89	Joback Method
cpg	792.16	J/mol×K	869.55	Joback Method
cpg	803.98	J/mol×K	902.20	Joback Method
cpg	814.97	J/mol×K	934.86	Joback Method
cpg	825.15	J/mol×K	967.51	Joback Method
cpg	834.56	J/mol×K	1000.17	Joback Method
dvisc	0.0006759	Pa×s	495.31	Joback Method

dvisc	0.0003669	Pa×s	546.80	Joback Method
dvisc	0.0002212	Pa×s	598.29	Joback Method
dvisc	0.0001445	Pa×s	649.77	Joback Method
dvisc	0.0001005	Pa×s	701.26	Joback Method
dvisc	0.0000735	Pa×s	752.75	Joback Method
dvisc	0.0000559	Pa×s	804.24	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=U353479&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