Glutaric acid, pentyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C12H19Cl3O4/c1-2-3-4-8-18-10(16)6-5-7-11(17)19-9-12(13,14)15/h2-9H2,1H3
InchiKey: VZGXOPJSKJDNSL-UHFFFAOYSA-N
Formula: C12H19Cl3O4
SMILES: CCCCCOC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 333.64

Physical Properties

Property code	Value	Unit	Source
gf	-450.63	kJ/mol	Joback Method
hf	-836.58	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.803		Crippen Method
mcvol	231.540	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	735.60	K	Joback Method
tc	933.37	K	Joback Method
tf	461.50	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.52	J/mol×K	735.60	Joback Method
cpg	613.90	J/mol×K	768.56	Joback Method
cpg	625.49	J/mol×K	801.52	Joback Method
cpg	636.31	J/mol×K	834.49	Joback Method
cpg	646.38	J/mol×K	867.45	Joback Method
cpg	655.72	J/mol×K	900.41	Joback Method
cpg	664.35	J/mol×K	933.37	Joback Method
dvisc	0.0009510	Pa×s	461.50	Joback Method

dvisc	0.0005367	Pa×s	507.18	Joback Method
dvisc	0.0003329	Pa×s	552.87	Joback Method
dvisc	0.0002221	Pa×s	598.55	Joback Method
dvisc	0.0001569	Pa×s	644.23	Joback Method
dvisc	0.0001161	Pa×s	689.92	Joback Method
dvisc	0.0000892	Pa×s	735.60	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=U359347&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