Glutaric acid, heptyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C14H23Cl3O4/c1-2-3-4-5-6-10-20-12(18)8-7-9-13(19)21-11-14(15,16)17/h2-11
InchiKey: OSNHVVNUMDFENK-UHFFFAOYSA-N
Formula: C14H23Cl3O4
SMILES: CCCCCCCOC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 361.69

Physical Properties

Property code	Value	Unit	Source
gf	-433.79	kJ/mol	Joback Method
hf	-877.86	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.584		Crippen Method
mcvol	259.720	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
tb	781.36	K	Joback Method
tc	977.33	K	Joback Method
tf	484.04	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.06	J/mol×K	781.36	Joback Method
cpg	723.27	J/mol×K	814.02	Joback Method
cpg	735.62	J/mol×K	846.68	Joback Method
cpg	747.14	J/mol×K	879.34	Joback Method
cpg	757.86	J/mol×K	912.00	Joback Method
cpg	767.79	J/mol×K	944.66	Joback Method
cpg	776.97	J/mol×K	977.33	Joback Method
dvisc	0.0007602	Pa×s	484.04	Joback Method

dvisc	0.0004178	Pa×s	533.59	Joback Method
dvisc	0.0002542	Pa×s	583.15	Joback Method
dvisc	0.0001672	Pa×s	632.70	Joback Method
dvisc	0.0001169	Pa×s	682.25	Joback Method
dvisc	0.0000857	Pa×s	731.81	Joback Method
dvisc	0.0000654	Pa×s	781.36	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=U359348&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