Glutaric acid, isobutyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C11H17Cl3O4/c1-8(2)6-17-9(15)4-3-5-10(16)18-7-11(12,13)14/h8H,3-7H2,1-2
InchiKey: ITWOXHYBQPUWBS-UHFFFAOYSA-N
Formula: C11H17Cl3O4
SMILES: CC(C)COC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 319.61

Physical Properties

Property code	Value	Unit	Source
gf	-461.49	kJ/mol	Joback Method
hf	-821.22	kJ/mol	Joback Method
hfus	31.47	kJ/mol	Joback Method
hvap	69.86	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.269		Crippen Method
mcvol	217.450	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	712.28	K	Joback Method
tc	914.88	K	Joback Method
tf	435.23	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.54	J/mol×K	712.28	Joback Method
cpg	602.34	J/mol×K	881.12	Joback Method
cpg	593.29	J/mol×K	847.35	Joback Method
cpg	583.50	J/mol×K	813.58	Joback Method
cpg	572.96	J/mol×K	779.81	Joback Method
cpg	561.65	J/mol×K	746.05	Joback Method
cpg	610.68	J/mol×K	914.88	Joback Method
dvisc	0.0000960	Pa×s	712.28	Joback Method

dvisc	0.0001270	Pa×s	666.11	Joback Method
dvisc	0.0001751	Pa×s	619.93	Joback Method
dvisc	0.0002543	Pa×s	573.75	Joback Method
dvisc	0.0003943	Pa×s	527.58	Joback Method
dvisc	0.0006651	Pa×s	481.41	Joback Method
dvisc	0.0012533	Pa×s	435.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359345&Units=SI
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

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