Glutaric acid, 2,2-dichloroethyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C11H12Cl2F6O4/c12-6(13)4-22-7(20)2-1-3-8(21)23-5-10(15,16)9(14)11(17,18

InchiKey: CWFRGEDIFVXCLX-UHFFFAOYSA-N

Formula: C11H12Cl2F6O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)C(F)(F)F)OCC(Cl)Cl

Mol. weight [g/mol]: 393.11

Physical Properties

Property code	Value	Unit	Source
gf	-1618.02	kJ/mol	Joback Method
hf	-1996.17	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	58.89	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.583		Crippen Method
mcvol	215.830	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
tb	666.80	K	Joback Method
tc	837.80	K	Joback Method
tf	396.27	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.87	J/mol×K	666.80	Joback Method
cpg	586.64	J/mol×K	695.30	Joback Method
cpg	596.74	J/mol×K	723.80	Joback Method
cpg	606.18	J/mol×K	752.30	Joback Method
cpg	615.01	J/mol×K	780.80	Joback Method
cpg	623.24	J/mol×K	809.30	Joback Method
cpg	630.89	J/mol×K	837.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393686&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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume