Glutaric acid, 2,4,6-trichlorophenyl 2-fluoroethyl ester

Inchi: InChI=1S/C13H12Cl3FO4/c14-8-6-9(15)13(10(16)7-8)21-12(19)3-1-2-11(18)20-5-4-17/h6

InchiKey: HLDUSYJSEVZBSG-UHFFFAOYSA-N

Formula: C13H12Cl3FO4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCCF

Mol. weight [g/mol]: 357.59

Physical Properties

Property code	Value	Unit	Source
gf	-556.34	kJ/mol	Joback Method
hf	-842.46	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	79.44	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.235		Crippen Method
mcvol	223.640	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	802.60	K	Joback Method
tc	1015.31	K	Joback Method
tf	534.92	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.61	J/mol×K	802.60	Joback Method
cpg	573.73	J/mol×K	838.05	Joback Method
cpg	583.01	J/mol×K	873.50	Joback Method
cpg	591.45	J/mol×K	908.96	Joback Method
cpg	599.05	J/mol×K	944.41	Joback Method
cpg	605.82	J/mol×K	979.86	Joback Method
cpg	611.74	J/mol×K	1015.31	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=U393719&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume