Glutaric acid, 2-chloro-6-fluorophenyl 2-fluoroethyl ester

Inchi: InChI=1S/C13H13ClF2O4/c14-9-3-1-4-10(16)13(9)20-12(18)6-2-5-11(17)19-8-7-15/h1,3-

InchiKey: WVKQWUUJVIOIFC-UHFFFAOYSA-N

Formula: C13H13ClF2O4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCCF

Mol. weight [g/mol]: 306.69

Physical Properties

Property code	Value	Unit	Source
gf	-717.66	kJ/mol	Joback Method
hf	-995.62	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	69.19	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.067		Crippen Method
mcvol	200.930	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	722.03	K	Joback Method
tc	919.72	K	Joback Method
tf	463.15	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.64	J/mol×K	722.03	Joback Method
cpg	539.34	J/mol×K	754.98	Joback Method
cpg	550.29	J/mol×K	787.93	Joback Method
cpg	560.48	J/mol×K	820.88	Joback Method
cpg	569.93	J/mol×K	853.83	Joback Method
cpg	578.63	J/mol×K	886.77	Joback Method
cpg	586.58	J/mol×K	919.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393714&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume