Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C14H12ClF5O4/c15-8-3-1-4-9(16)12(8)24-11(22)6-2-5-10(21)23-7-14(19,20)13

InchiKey: WBTOVAUWPFHTJU-UHFFFAOYSA-N

Formula: C14H12ClF5O4

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

Mol. weight [g/mol]: 374.69

Physical Properties

Property code	Value	Unit	Source
gf	-1293.27	kJ/mol	Joback Method
hf	-1618.62	kJ/mol	Joback Method
hfus	39.51	kJ/mol	Joback Method
hvap	67.29	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.998		Crippen Method
mcvol	220.330	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
tb	739.05	K	Joback Method
tc	927.28	K	Joback Method
tf	463.61	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.93	J/mol×K	739.05	Joback Method
cpg	618.11	J/mol×K	770.42	Joback Method
cpg	628.52	J/mol×K	801.79	Joback Method
cpg	638.17	J/mol×K	833.16	Joback Method
cpg	647.09	J/mol×K	864.54	Joback Method
cpg	655.30	J/mol×K	895.91	Joback Method
cpg	662.81	J/mol×K	927.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391576&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