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

Inchi: InChI=1S/C14H11ClF6O4/c15-8-3-1-4-9(16)12(8)25-11(23)6-2-5-10(22)24-7-13(17,18)14

InchiKey: RXQFNBVOADVANF-UHFFFAOYSA-N

Formula: C14H11ClF6O4

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

Mol. weight [g/mol]: 392.68

Physical Properties

Property code	Value	Unit	Source
gf	-1482.80	kJ/mol	Joback Method
hf	-1818.20	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	65.56	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.296		Crippen Method
mcvol	222.100	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	735.53	K	Joback Method
tc	922.41	K	Joback Method
tf	481.62	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.74	J/mol×K	735.53	Joback Method
cpg	627.50	J/mol×K	766.68	Joback Method
cpg	637.47	J/mol×K	797.82	Joback Method
cpg	646.71	J/mol×K	828.97	Joback Method
cpg	655.23	J/mol×K	860.12	Joback Method
cpg	663.07	J/mol×K	891.26	Joback Method
cpg	670.28	J/mol×K	922.41	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=U393675&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