Glutaric acid, 2-chloro-6-fluorophenyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C15H12ClF7O4/c16-8-3-1-4-9(17)12(8)27-11(25)6-2-5-10(24)26-7-14(19,20)13

InchiKey: YWLVECCSHCFVFP-UHFFFAOYSA-N

Formula: C15H12ClF7O4

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

Mol. weight [g/mol]: 424.69

Physical Properties

Property code	Value	Unit	Source
gf	-1671.63	kJ/mol	Joback Method
hf	-2040.23	kJ/mol	Joback Method
hfus	40.85	kJ/mol	Joback Method
hvap	66.58	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.634		Crippen Method
mcvol	237.960	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	1857.00		NIST Webbook
tb	757.24	K	Joback Method
tc	941.48	K	Joback Method
tf	478.48	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.11	J/mol×K	757.24	Joback Method
cpg	689.07	J/mol×K	787.95	Joback Method
cpg	699.22	J/mol×K	818.65	Joback Method
cpg	708.62	J/mol×K	849.36	Joback Method
cpg	717.29	J/mol×K	880.07	Joback Method
cpg	725.26	J/mol×K	910.77	Joback Method
cpg	732.59	J/mol×K	941.48	Joback Method

Sources

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=U393692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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