Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-chlorophenyl ester

Inchi: InChI=1S/C14H13ClF4O4/c15-9-4-1-2-5-10(9)23-12(21)7-3-6-11(20)22-8-14(18,19)13(16

InchiKey: QDWGWOFUUGGLMK-UHFFFAOYSA-N

Formula: C14H13ClF4O4

SMILES: O=C(CCCC(=O)Oc1ccccc1Cl)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 356.70

Physical Properties

Property code	Value	Unit	Source
gf	-1088.83	kJ/mol	Joback Method
hf	-1411.04	kJ/mol	Joback Method
hfus	36.82	kJ/mol	Joback Method
hvap	67.44	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.859		Crippen Method
mcvol	218.560	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	734.80	K	Joback Method
tc	927.93	K	Joback Method
tf	450.50	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.33	J/mol×K	734.80	Joback Method
cpg	612.04	J/mol×K	766.99	Joback Method
cpg	622.92	J/mol×K	799.18	Joback Method
cpg	633.00	J/mol×K	831.36	Joback Method
cpg	642.29	J/mol×K	863.55	Joback Method
cpg	650.83	J/mol×K	895.74	Joback Method
cpg	658.64	J/mol×K	927.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391881&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