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

Inchi: InChI=1S/C14H12ClF5O4/c15-9-3-1-4-10(7-9)24-12(22)6-2-5-11(21)23-8-13(16,17)14(18

InchiKey: GUKGAIMHNWUGCN-UHFFFAOYSA-N

Formula: C14H12ClF5O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 374.69

Physical Properties

Property code	Value	Unit	Source
gf	-1278.36	kJ/mol	Joback Method
hf	-1610.62	kJ/mol	Joback Method
hfus	36.01	kJ/mol	Joback Method
hvap	65.72	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.156		Crippen Method
mcvol	220.330	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
tb	731.28	K	Joback Method
tc	922.97	K	Joback Method
tf	468.51	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.17	J/mol×K	731.28	Joback Method
cpg	621.44	J/mol×K	763.23	Joback Method
cpg	631.88	J/mol×K	795.18	Joback Method
cpg	641.52	J/mol×K	827.12	Joback Method
cpg	650.40	J/mol×K	859.07	Joback Method
cpg	658.57	J/mol×K	891.02	Joback Method
cpg	666.07	J/mol×K	922.97	Joback Method

Sources

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=U393676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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