Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C15H15ClF4O4/c1-9-7-10(16)5-6-11(9)24-13(22)4-2-3-12(21)23-8-15(19,20)14

InchiKey: BYFLKPSOXDYWEO-UHFFFAOYSA-N

Formula: C15H15ClF4O4

SMILES: Cc1cc(Cl)ccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 370.72

Physical Properties

Property code	Value	Unit	Source
gf	-1090.04	kJ/mol	Joback Method
hf	-1443.15	kJ/mol	Joback Method
hfus	39.02	kJ/mol	Joback Method
hvap	70.33	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.168		Crippen Method
mcvol	232.650	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2018.00		NIST Webbook
rinpol	2018.00		NIST Webbook
tb	762.66	K	Joback Method
tc	955.90	K	Joback Method
tf	474.29	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.58	J/mol×K	762.66	Joback Method
cpg	664.59	J/mol×K	794.87	Joback Method
cpg	675.76	J/mol×K	827.07	Joback Method
cpg	686.10	J/mol×K	859.28	Joback Method
cpg	695.64	J/mol×K	891.49	Joback Method
cpg	704.40	J/mol×K	923.69	Joback Method
cpg	712.40	J/mol×K	955.90	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=U392062&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