Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C15H16ClF3O4/c1-9-8-11(16)6-7-12(9)23-14(21)5-3-4-13(20)22-10(2)15(17,18

InchiKey: RMEBXRVNMDUFBQ-UHFFFAOYSA-N

Formula: C15H16ClF3O4

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

Mol. weight [g/mol]: 352.73

Physical Properties

Property code	Value	Unit	Source
gf	-895.23	kJ/mol	Joback Method
hf	-1247.04	kJ/mol	Joback Method
hfus	35.94	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.218		Crippen Method
mcvol	230.880	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	763.39	K	Joback Method
tc	962.40	K	Joback Method
tf	473.70	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.84	J/mol×K	763.39	Joback Method
cpg	657.30	J/mol×K	796.56	Joback Method
cpg	668.87	J/mol×K	829.73	Joback Method
cpg	679.57	J/mol×K	862.90	Joback Method
cpg	689.42	J/mol×K	896.06	Joback Method
cpg	698.46	J/mol×K	929.23	Joback Method
cpg	706.70	J/mol×K	962.40	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=U392061&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