Glutaric acid, 1,1,1-trifluoroprop-2-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C15H16ClF3O5/c1-9(15(17,18)19)23-13(20)4-3-5-14(21)24-11-7-6-10(16)8-12

InchiKey: QZIXQOAYHINRTO-UHFFFAOYSA-N

Formula: C15H16ClF3O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 368.73

Physical Properties

Property code	Value	Unit	Source
gf	-1000.23	kJ/mol	Joback Method
hf	-1379.26	kJ/mol	Joback Method
hfus	37.13	kJ/mol	Joback Method
hvap	73.56	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.918		Crippen Method
mcvol	236.750	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook
tb	785.81	K	Joback Method
tc	984.61	K	Joback Method
tf	495.93	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.15	J/mol×K	785.81	Joback Method
cpg	683.29	J/mol×K	818.94	Joback Method
cpg	694.51	J/mol×K	852.08	Joback Method
cpg	704.81	J/mol×K	885.21	Joback Method
cpg	714.21	J/mol×K	918.34	Joback Method
cpg	722.72	J/mol×K	951.48	Joback Method
cpg	730.36	J/mol×K	984.61	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=U393899&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