Glutaric acid, 2,2,3,3-tetrafluoropropyl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C15H15ClF4O5/c1-23-11-7-9(16)5-6-10(11)25-13(22)4-2-3-12(21)24-8-15(19,2

InchiKey: XIJSRLDPFJUGCZ-UHFFFAOYSA-N

Formula: C15H15ClF4O5

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

Mol. weight [g/mol]: 386.72

Physical Properties

Property code	Value	Unit	Source
gf	-1195.04	kJ/mol	Joback Method
hf	-1575.37	kJ/mol	Joback Method
hfus	40.21	kJ/mol	Joback Method
hvap	72.74	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.868		Crippen Method
mcvol	238.520	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
tb	785.08	K	Joback Method
tc	978.67	K	Joback Method
tf	496.52	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.81	J/mol×K	785.08	Joback Method
cpg	690.55	J/mol×K	817.35	Joback Method
cpg	701.40	J/mol×K	849.61	Joback Method
cpg	711.38	J/mol×K	881.88	Joback Method
cpg	720.50	J/mol×K	914.14	Joback Method
cpg	728.77	J/mol×K	946.41	Joback Method
cpg	736.22	J/mol×K	978.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393900&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