Glutaric acid, 2,2,3,3-tetrafluoropropyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C14H11Cl3F4O4/c15-7-4-8(16)12(17)9(5-7)25-11(23)3-1-2-10(22)24-6-14(20,2

InchiKey: OMMFJMSTXWARPJ-UHFFFAOYSA-N

Formula: C14H11Cl3F4O4

SMILES: O=C(CCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 425.59

Physical Properties

Property code	Value	Unit	Source
gf	-1131.95	kJ/mol	Joback Method
hf	-1465.46	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.166		Crippen Method
mcvol	243.040	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tb	819.62	K	Joback Method
tc	1022.92	K	Joback Method
tf	535.38	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.56	J/mol×K	819.62	Joback Method
cpg	652.07	J/mol×K	853.50	Joback Method
cpg	660.77	J/mol×K	887.39	Joback Method
cpg	668.67	J/mol×K	921.27	Joback Method
cpg	675.80	J/mol×K	955.15	Joback Method
cpg	682.18	J/mol×K	989.04	Joback Method
cpg	687.84	J/mol×K	1022.92	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392173&Units=SI

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