Glutaric acid, 3-chlorophenyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C17H12ClF3O4/c18-10-3-1-4-11(9-10)24-14(22)5-2-6-15(23)25-13-8-7-12(19)

InchiKey: CIDURGJEPFTBGM-UHFFFAOYSA-N

Formula: C17H12ClF3O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)c(F)c1F)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 372.72

Physical Properties

Property code	Value	Unit	Source
gf	-785.64	kJ/mol	Joback Method
hf	-1060.70	kJ/mol	Joback Method
hfus	45.32	kJ/mol	Joback Method
hvap	80.88	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.439		Crippen Method
mcvol	235.300	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	2401.00		NIST Webbook
rinpol	2401.00		NIST Webbook
tb	849.46	K	Joback Method
tc	1064.58	K	Joback Method
tf	560.28	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.68	J/mol×K	849.46	Joback Method
cpg	664.35	J/mol×K	885.31	Joback Method
cpg	674.00	J/mol×K	921.17	Joback Method
cpg	682.64	J/mol×K	957.02	Joback Method
cpg	690.28	J/mol×K	992.88	Joback Method
cpg	696.93	J/mol×K	1028.73	Joback Method
cpg	702.61	J/mol×K	1064.58	Joback Method

Sources

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=U393643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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