Glutaric acid, 2,4,6-trichlorophenyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C18H11Cl3F4O4/c19-9-7-11(20)17(12(21)8-9)29-15(27)6-2-5-14(26)28-13-4-1

InchiKey: GVQIEWLTRYRNEQ-UHFFFAOYSA-N

Formula: C18H11Cl3F4O4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 473.63

Physical Properties

Property code	Value	Unit	Source
gf	-1002.68	kJ/mol	Joback Method
hf	-1329.15	kJ/mol	Joback Method
hfus	51.58	kJ/mol	Joback Method
hvap	90.43	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	6.486		Crippen Method
mcvol	275.640	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	948.22	K	Joback Method
tc	1173.18	K	Joback Method
tf	646.92	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.24	J/mol×K	948.22	Joback Method
cpg	762.45	J/mol×K	985.71	Joback Method
cpg	769.66	J/mol×K	1023.21	Joback Method
cpg	775.89	J/mol×K	1060.70	Joback Method
cpg	781.20	J/mol×K	1098.19	Joback Method
cpg	785.63	J/mol×K	1135.68	Joback Method
cpg	789.20	J/mol×K	1173.18	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=U393626&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