Glutaric acid, 2,4,6-trichlorophenyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C17H11Cl4FO4/c18-9-7-11(20)16(12(21)8-9)25-14(23)5-2-6-15(24)26-17-10(1

InchiKey: SREXNFXJQVWXAV-UHFFFAOYSA-N

Formula: C17H11Cl4FO4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 440.08

Physical Properties

Property code	Value	Unit	Source
gf	-441.44	kJ/mol	Joback Method
hf	-727.17	kJ/mol	Joback Method
hfus	51.37	kJ/mol	Joback Method
hvap	96.33	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.121		Crippen Method
mcvol	268.480	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	2898.00		NIST Webbook
rinpol	2898.00		NIST Webbook
tb	968.19	K	Joback Method
tc	1207.34	K	Joback Method
tf	661.38	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.18	J/mol×K	968.19	Joback Method
cpg	700.75	J/mol×K	1008.05	Joback Method
cpg	707.14	J/mol×K	1047.91	Joback Method
cpg	712.36	J/mol×K	1087.76	Joback Method
cpg	716.42	J/mol×K	1127.62	Joback Method
cpg	719.34	J/mol×K	1167.48	Joback Method
cpg	721.13	J/mol×K	1207.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391591&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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