Glutaric acid, 2,3-dichlorophenyl 3-fluorophenyl ester

Inchi: InChI=1S/C17H13Cl2FO4/c18-13-6-2-7-14(17(13)19)24-16(22)9-3-8-15(21)23-12-5-1-4-1

InchiKey: VPNNHNJMYQCDPS-UHFFFAOYSA-N

Formula: C17H13Cl2FO4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)Oc1cccc(F)c1

Mol. weight [g/mol]: 371.19

Physical Properties

Property code	Value	Unit	Source
gf	-398.32	kJ/mol	Joback Method
hf	-672.75	kJ/mol	Joback Method
hfus	43.75	kJ/mol	Joback Method
hvap	86.24	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.814		Crippen Method
mcvol	244.000	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook
tb	883.37	K	Joback Method
tc	1114.35	K	Joback Method
tf	576.50	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.94	J/mol×K	883.37	Joback Method
cpg	671.30	J/mol×K	921.87	Joback Method
cpg	680.53	J/mol×K	960.36	Joback Method
cpg	688.63	J/mol×K	998.86	Joback Method
cpg	695.64	J/mol×K	1037.36	Joback Method
cpg	701.57	J/mol×K	1075.86	Joback Method
cpg	706.44	J/mol×K	1114.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392097&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