Glutaric acid, 2,3-dichlorophenyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C17H12Cl3FO4/c18-10-4-2-7-13(16(10)20)24-14(22)8-3-9-15(23)25-17-11(19)5-1-6-12(17)21

InchiKey: YSIKIMUXAYGNGT-UHFFFAOYSA-N

Formula: C17H12Cl3FO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 405.63

Physical Properties

Property code	Value	Unit	Source
gf	-419.88	kJ/mol	Joback Method
hf	-699.96	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	91.29	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.467		Crippen Method
mcvol	256.240	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	2781.00		NIST Webbook
rinpol	2781.00		NIST Webbook
tb	925.78	K	Joback Method
tc	1160.71	K	Joback Method
tf	618.94	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.05	J/mol×K	925.78	Joback Method
cpg	687.03	J/mol×K	964.94	Joback Method
cpg	694.85	J/mol×K	1004.09	Joback Method
cpg	701.53	J/mol×K	1043.25	Joback Method
cpg	707.10	J/mol×K	1082.40	Joback Method
cpg	711.56	J/mol×K	1121.56	Joback Method
cpg	714.94	J/mol×K	1160.71	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=U391589&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