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

Inchi: InChI=1S/C17H11Cl2F3O4/c18-9-3-1-4-11(15(9)19)25-13(23)5-2-6-14(24)26-12-8-7-10(

InchiKey: OEDRMJKIAVZHMC-UHFFFAOYSA-N

Formula: C17H11Cl2F3O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 407.17

Physical Properties

Property code	Value	Unit	Source
gf	-807.20	kJ/mol	Joback Method
hf	-1087.91	kJ/mol	Joback Method
hfus	49.13	kJ/mol	Joback Method
hvap	85.93	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.092		Crippen Method
mcvol	247.540	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	2617.00		NIST Webbook
rinpol	2617.00		NIST Webbook
tb	891.87	K	Joback Method
tc	1111.76	K	Joback Method
tf	602.72	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.20	J/mol×K	891.87	Joback Method
cpg	681.60	J/mol×K	928.52	Joback Method
cpg	689.94	J/mol×K	965.17	Joback Method
cpg	697.25	J/mol×K	1001.82	Joback Method
cpg	703.53	J/mol×K	1038.46	Joback Method
cpg	708.77	J/mol×K	1075.11	Joback Method
cpg	713.00	J/mol×K	1111.76	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=U393645&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