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

Inchi: InChI=1S/C18H15Cl2FO4/c19-13-9-7-12(8-10-13)11-24-16(22)5-2-6-17(23)25-18-14(20)
InchiKey: VSZIRJITQKFPCR-UHFFFAOYSA-N
Formula: C18H15Cl2FO4
SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCc1ccc(Cl)cc1
Mol. weight [g/mol]: 385.21

Physical Properties

Property code	Value	Unit	Source
gf	-389.90	kJ/mol	Joback Method
hf	-693.39	kJ/mol	Joback Method
hfus	46.34	kJ/mol	Joback Method
hvap	88.46	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.952		Crippen Method
mcvol	258.090	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	906.25	K	Joback Method
tc	1135.33	K	Joback Method
tf	587.77	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.60	J/mol×K	906.25	Joback Method
cpg	727.16	J/mol×K	944.43	Joback Method
cpg	736.55	J/mol×K	982.61	Joback Method
cpg	744.79	J/mol×K	1020.79	Joback Method
cpg	751.92	J/mol×K	1058.97	Joback Method
cpg	757.94	J/mol×K	1097.15	Joback Method
cpg	762.90	J/mol×K	1135.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391731&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

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