Glutaric acid, 2-chloro-6-fluorophenyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C18H24ClFO4/c1-11(2)17(12(3)4)23-15(21)9-6-10-16(22)24-18-13(19)7-5-8-14

InchiKey: LANLXQHAKBVLPL-UHFFFAOYSA-N

Formula: C18H24ClFO4

SMILES: CC(C)C(OC(=O)CCCC(=O)Oc1c(F)cccc1Cl)C(C)C

Mol. weight [g/mol]: 358.83

Physical Properties

Property code	Value	Unit	Source
gf	-488.07	kJ/mol	Joback Method
hf	-918.55	kJ/mol	Joback Method
hfus	37.92	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.779		Crippen Method
mcvol	269.610	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	835.84	K	Joback Method
tc	1042.14	K	Joback Method
tf	473.91	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.53	J/mol×K	835.84	Joback Method
cpg	810.93	J/mol×K	870.22	Joback Method
cpg	824.21	J/mol×K	904.61	Joback Method
cpg	836.40	J/mol×K	938.99	Joback Method
cpg	847.49	J/mol×K	973.37	Joback Method
cpg	857.52	J/mol×K	1007.75	Joback Method
cpg	866.50	J/mol×K	1042.14	Joback Method

Sources

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=U393480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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