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

Inchi: InChI=1S/C19H18ClFO5/c1-24-14-10-8-13(9-11-14)12-25-17(22)6-3-7-18(23)26-19-15(2

InchiKey: KDVGOAOJTWOAIZ-UHFFFAOYSA-N

Formula: C19H18ClFO5

SMILES: COc1ccc(COC(=O)CCCC(=O)Oc2c(F)cccc2Cl)cc1

Mol. weight [g/mol]: 380.80

Physical Properties

Property code	Value	Unit	Source
gf	-474.55	kJ/mol	Joback Method
hf	-830.51	kJ/mol	Joback Method
hfus	45.92	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.307		Crippen Method
mcvol	265.810	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	914.12	K	Joback Method
tc	1137.85	K	Joback Method
tf	591.35	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.15	J/mol×K	914.12	Joback Method
cpg	789.47	J/mol×K	951.41	Joback Method
cpg	799.49	J/mol×K	988.70	Joback Method
cpg	808.20	J/mol×K	1025.99	Joback Method
cpg	815.62	J/mol×K	1063.27	Joback Method
cpg	821.75	J/mol×K	1100.56	Joback Method
cpg	826.60	J/mol×K	1137.85	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=U391745&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