Glutaric acid, 2-chloro-6-fluorophenyl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C19H18ClFO5/c1-12-9-10-15(24-2)16(11-12)25-17(22)7-4-8-18(23)26-19-13(2

InchiKey: QJSTXHCIRSXOCW-UHFFFAOYSA-N

Formula: C19H18ClFO5

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 380.80

Physical Properties

Property code	Value	Unit	Source
gf	-484.18	kJ/mol	Joback Method
hf	-841.98	kJ/mol	Joback Method
hfus	45.53	kJ/mol	Joback Method
hvap	89.38	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.477		Crippen Method
mcvol	265.810	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	919.10	K	Joback Method
tc	1143.62	K	Joback Method
tf	603.87	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.66	J/mol×K	919.10	Joback Method
cpg	787.87	J/mol×K	956.52	Joback Method
cpg	797.75	J/mol×K	993.94	Joback Method
cpg	806.30	J/mol×K	1031.36	Joback Method
cpg	813.51	J/mol×K	1068.78	Joback Method
cpg	819.39	J/mol×K	1106.20	Joback Method
cpg	823.95	J/mol×K	1143.62	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=U393929&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