Glutaric acid, 2-chloro-6-fluorophenyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C18H15BrClFO5/c1-24-15-10-11(19)8-9-14(15)25-16(22)6-3-7-17(23)26-18-12

InchiKey: YILCDVFVMLKWRN-UHFFFAOYSA-N

Formula: C18H15BrClFO5

SMILES: COc1cc(Br)ccc1OC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 445.66

Physical Properties

Property code	Value	Unit	Source
gf	-478.28	kJ/mol	Joback Method
hf	-795.01	kJ/mol	Joback Method
hfus	48.23	kJ/mol	Joback Method
hvap	93.59	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	4.931		Crippen Method
mcvol	269.220	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2943.00		NIST Webbook
rinpol	2943.00		NIST Webbook
tb	962.38	K	Joback Method
tc	1197.75	K	Joback Method
tf	652.40	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.97	J/mol×K	962.38	Joback Method
cpg	757.05	J/mol×K	1001.61	Joback Method
cpg	764.82	J/mol×K	1040.84	Joback Method
cpg	771.30	J/mol×K	1080.07	Joback Method
cpg	776.47	J/mol×K	1119.29	Joback Method
cpg	780.36	J/mol×K	1158.52	Joback Method
cpg	782.97	J/mol×K	1197.75	Joback Method

Sources

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=U393891&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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