Glutaric acid, 2-fluorophenyl 4-bromophenyl ester

Inchi: InChI=1S/C17H14BrFO4/c18-12-8-10-13(11-9-12)22-16(20)6-3-7-17(21)23-15-5-2-1-4-14

InchiKey: GWMHGJJTTLXEKE-UHFFFAOYSA-N

Formula: C17H14BrFO4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 381.19

Physical Properties

Property code	Value	Unit	Source
gf	-350.51	kJ/mol	Joback Method
hf	-603.47	kJ/mol	Joback Method
hfus	41.03	kJ/mol	Joback Method
hvap	83.24	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.269		Crippen Method
mcvol	237.020	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook
tb	869.69	K	Joback Method
tc	1103.32	K	Joback Method
tf	563.94	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.35	J/mol×K	869.69	Joback Method
cpg	662.54	J/mol×K	908.63	Joback Method
cpg	672.60	J/mol×K	947.57	Joback Method
cpg	681.57	J/mol×K	986.51	Joback Method
cpg	689.47	J/mol×K	1025.45	Joback Method
cpg	696.36	J/mol×K	1064.39	Joback Method
cpg	702.26	J/mol×K	1103.32	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393292&Units=SI

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