Glutaric acid, 2-fluorophenyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C17H13BrF2O4/c18-12-10-11(19)8-9-14(12)23-16(21)6-3-7-17(22)24-15-5-2-1

InchiKey: QQKFXUVHIHZLJG-UHFFFAOYSA-N

Formula: C17H13BrF2O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)cc1Br)Oc1ccccc1F

Mol. weight [g/mol]: 399.18

Physical Properties

Property code	Value	Unit	Source
gf	-554.95	kJ/mol	Joback Method
hf	-811.05	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	83.09	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.409		Crippen Method
mcvol	238.790	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	2496.00		NIST Webbook
rinpol	2496.00		NIST Webbook
tb	873.94	K	Joback Method
tc	1101.01	K	Joback Method
tf	577.05	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.12	J/mol×K	873.94	Joback Method
cpg	667.77	J/mol×K	911.78	Joback Method
cpg	677.33	J/mol×K	949.63	Joback Method
cpg	685.86	J/mol×K	987.47	Joback Method
cpg	693.36	J/mol×K	1025.32	Joback Method
cpg	699.88	J/mol×K	1063.16	Joback Method
cpg	705.43	J/mol×K	1101.01	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=U390206&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