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

Inchi: InChI=1S/C17H12BrClF2O4/c18-11-9-10(20)7-8-14(11)24-15(22)5-2-6-16(23)25-17-12(1

InchiKey: ZRNQKGBLGDWOPW-UHFFFAOYSA-N

Formula: C17H12BrClF2O4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 433.63

Physical Properties

Property code	Value	Unit	Source
gf	-576.51	kJ/mol	Joback Method
hf	-838.26	kJ/mol	Joback Method
hfus	47.53	kJ/mol	Joback Method
hvap	88.13	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.062		Crippen Method
mcvol	251.030	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	2648.00		NIST Webbook
rinpol	2648.00		NIST Webbook
tb	916.35	K	Joback Method
tc	1147.55	K	Joback Method
tf	619.49	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.80	J/mol×K	916.35	Joback Method
cpg	684.13	J/mol×K	954.88	Joback Method
cpg	692.38	J/mol×K	993.42	Joback Method
cpg	699.58	J/mol×K	1031.95	Joback Method
cpg	705.75	J/mol×K	1070.48	Joback Method
cpg	710.91	J/mol×K	1109.02	Joback Method
cpg	715.09	J/mol×K	1147.55	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=U391834&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