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

Inchi: InChI=1S/C17H11BrCl3FO4/c18-11-8-10(22)4-5-14(11)25-15(23)2-1-3-16(24)26-17-12(2

InchiKey: YBAKLUPCFWJZBV-UHFFFAOYSA-N

Formula: C17H11BrCl3FO4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 484.53

Physical Properties

Property code	Value	Unit	Source
gf	-415.19	kJ/mol	Joback Method
hf	-685.10	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	98.38	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	6.230		Crippen Method
mcvol	273.740	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	996.92	K	Joback Method
tc	1242.12	K	Joback Method
tf	691.26	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.54	J/mol×K	996.92	Joback Method
cpg	706.64	J/mol×K	1037.79	Joback Method
cpg	712.60	J/mol×K	1078.65	Joback Method
cpg	717.44	J/mol×K	1119.52	Joback Method
cpg	721.19	J/mol×K	1160.38	Joback Method
cpg	723.87	J/mol×K	1201.25	Joback Method
cpg	725.50	J/mol×K	1242.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391839&Units=SI
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

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