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

Inchi: InChI=1S/C17H13BrClFO4/c18-11-7-9-12(10-8-11)23-15(21)5-2-6-16(22)24-17-13(19)3-

InchiKey: MMRFYCGEMSVNCC-UHFFFAOYSA-N

Formula: C17H13BrClFO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 415.64

Physical Properties

Property code	Value	Unit	Source
gf	-372.07	kJ/mol	Joback Method
hf	-630.68	kJ/mol	Joback Method
hfus	44.84	kJ/mol	Joback Method
hvap	88.29	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	4.923		Crippen Method
mcvol	249.260	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		NIST Webbook
tb	912.10	K	Joback Method
tc	1149.35	K	Joback Method
tf	606.38	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.34	J/mol×K	912.10	Joback Method
cpg	679.16	J/mol×K	951.64	Joback Method
cpg	687.86	J/mol×K	991.18	Joback Method
cpg	695.47	J/mol×K	1030.72	Joback Method
cpg	702.03	J/mol×K	1070.27	Joback Method
cpg	707.56	J/mol×K	1109.81	Joback Method
cpg	712.10	J/mol×K	1149.35	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=U393295&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