Glutaric acid, 2,3-dichlorophenyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C17H12BrCl2FO4/c18-11-9-10(21)7-8-13(11)24-15(22)5-2-6-16(23)25-14-4-1-

InchiKey: PMJDZFFGIJBJAU-UHFFFAOYSA-N

Formula: C17H12BrCl2FO4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 450.08

Physical Properties

Property code	Value	Unit	Source
gf	-393.63	kJ/mol	Joback Method
hf	-657.89	kJ/mol	Joback Method
hfus	48.65	kJ/mol	Joback Method
hvap	93.34	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	5.576		Crippen Method
mcvol	261.500	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	2935.00		NIST Webbook
rinpol	2935.00		NIST Webbook
tb	954.51	K	Joback Method
tc	1195.58	K	Joback Method
tf	648.82	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.38	J/mol×K	954.51	Joback Method
cpg	693.85	J/mol×K	994.69	Joback Method
cpg	701.19	J/mol×K	1034.87	Joback Method
cpg	707.43	J/mol×K	1075.05	Joback Method
cpg	712.61	J/mol×K	1115.22	Joback Method
cpg	716.75	J/mol×K	1155.40	Joback Method
cpg	719.88	J/mol×K	1195.58	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=U391837&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