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

Inchi: InChI=1S/C18H16BrFO5/c1-23-16-11-12(19)9-10-15(16)25-18(22)8-4-7-17(21)24-14-6-3

InchiKey: KFQSWCAOTWPLHN-UHFFFAOYSA-N

Formula: C18H16BrFO5

SMILES: COc1cc(Br)ccc1OC(=O)CCCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 411.22

Physical Properties

Property code	Value	Unit	Source
gf	-456.72	kJ/mol	Joback Method
hf	-767.80	kJ/mol	Joback Method
hfus	44.42	kJ/mol	Joback Method
hvap	88.54	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.278		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook
tb	919.97	K	Joback Method
tc	1150.85	K	Joback Method
tf	609.96	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.86	J/mol×K	919.97	Joback Method
cpg	741.46	J/mol×K	958.45	Joback Method
cpg	750.78	J/mol×K	996.93	Joback Method
cpg	758.85	J/mol×K	1035.41	Joback Method
cpg	765.67	J/mol×K	1073.89	Joback Method
cpg	771.26	J/mol×K	1112.37	Joback Method
cpg	775.63	J/mol×K	1150.85	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=U393888&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

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