Glutaric acid, 2-methylpent-3-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C17H22BrFO4/c1-4-14(11(2)3)22-16(20)6-5-7-17(21)23-15-9-8-12(19)10-13(1

InchiKey: SKSXNXQLQIQWRO-UHFFFAOYSA-N

Formula: C17H22BrFO4

SMILES: CCC(OC(=O)CCCC(=O)Oc1ccc(F)cc1Br)C(C)C

Mol. weight [g/mol]: 389.26

Physical Properties

Property code	Value	Unit	Source
gf	-467.80	kJ/mol	Joback Method
hf	-850.56	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.642		Crippen Method
mcvol	260.780	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
tb	842.13	K	Joback Method
tc	1052.89	K	Joback Method
tf	507.52	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.46	J/mol×K	842.13	Joback Method
cpg	764.97	J/mol×K	877.26	Joback Method
cpg	777.43	J/mol×K	912.38	Joback Method
cpg	788.85	J/mol×K	947.51	Joback Method
cpg	799.25	J/mol×K	982.64	Joback Method
cpg	808.66	J/mol×K	1017.76	Joback Method
cpg	817.09	J/mol×K	1052.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391826&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