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

Inchi: InChI=1S/C16H20BrFO4/c1-10(2)11(3)21-15(19)5-4-6-16(20)22-14-8-7-12(18)9-13(14)1

InchiKey: UHYGSNLXLWOMPY-UHFFFAOYSA-N

Formula: C16H20BrFO4

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

Mol. weight [g/mol]: 375.23

Physical Properties

Property code	Value	Unit	Source
gf	-476.22	kJ/mol	Joback Method
hf	-829.92	kJ/mol	Joback Method
hfus	37.35	kJ/mol	Joback Method
hvap	77.96	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.252		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2154.00		NIST Webbook
rinpol	2154.00		NIST Webbook
tb	819.25	K	Joback Method
tc	1031.09	K	Joback Method
tf	496.25	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.13	J/mol×K	819.25	Joback Method
cpg	708.39	J/mol×K	854.56	Joback Method
cpg	720.62	J/mol×K	889.86	Joback Method
cpg	731.86	J/mol×K	925.17	Joback Method
cpg	742.11	J/mol×K	960.48	Joback Method
cpg	751.39	J/mol×K	995.79	Joback Method
cpg	759.72	J/mol×K	1031.09	Joback Method

Sources

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=U391825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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