Glutaric acid, 2-bromo-5-fluorobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H26BrFO4/c1-4-6-17(13(2)3)25-19(23)8-5-7-18(22)24-12-14-11-15(21)9-1

InchiKey: KAZNWARUKOQVGU-UHFFFAOYSA-N

Formula: C19H26BrFO4

SMILES: CCCC(OC(=O)CCCC(=O)OCc1cc(F)ccc1Br)C(C)C

Mol. weight [g/mol]: 417.31

Physical Properties

Property code	Value	Unit	Source
gf	-450.96	kJ/mol	Joback Method
hf	-891.84	kJ/mol	Joback Method
hfus	45.12	kJ/mol	Joback Method
hvap	84.64	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.170		Crippen Method
mcvol	288.960	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	887.89	K	Joback Method
tc	1098.53	K	Joback Method
tf	530.06	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.62	J/mol×K	887.89	Joback Method
cpg	880.56	J/mol×K	923.00	Joback Method
cpg	893.37	J/mol×K	958.10	Joback Method
cpg	905.07	J/mol×K	993.21	Joback Method
cpg	915.69	J/mol×K	1028.32	Joback Method
cpg	925.25	J/mol×K	1063.43	Joback Method
cpg	933.78	J/mol×K	1098.53	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=U377064&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