Glutaric acid, 2-bromo-5-fluorobenzyl isobutyl ester

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

InchiKey: QZGJDOKIYDETMJ-UHFFFAOYSA-N

Formula: C16H20BrFO4

SMILES: CC(C)COC(=O)CCCC(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 375.23

Physical Properties

Property code	Value	Unit	Source
gf	-473.78	kJ/mol	Joback Method
hf	-824.64	kJ/mol	Joback Method
hfus	40.88	kJ/mol	Joback Method
hvap	78.35	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.001		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	819.69	K	Joback Method
tc	1028.89	K	Joback Method
tf	511.25	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.55	J/mol×K	819.69	Joback Method
cpg	707.66	J/mol×K	854.56	Joback Method
cpg	719.78	J/mol×K	889.42	Joback Method
cpg	730.93	J/mol×K	924.29	Joback Method
cpg	741.13	J/mol×K	959.16	Joback Method
cpg	750.40	J/mol×K	994.03	Joback Method
cpg	758.75	J/mol×K	1028.89	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=U377060&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