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

Inchi: InChI=1S/C16H20BrFO4/c1-2-3-9-21-15(19)5-4-6-16(20)22-11-12-10-13(18)7-8-14(12)1
InchiKey: LTLUQQSMDUOANH-UHFFFAOYSA-N
Formula: C16H20BrFO4
SMILES: CCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]: 375.23

Physical Properties

Property code	Value	Unit	Source
gf	-471.34	kJ/mol	Joback Method
hf	-819.36	kJ/mol	Joback Method
hfus	44.40	kJ/mol	Joback Method
hvap	78.74	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.145		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	820.13	K	Joback Method
tc	1026.85	K	Joback Method
tf	526.25	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.98	J/mol×K	820.13	Joback Method
cpg	706.94	J/mol×K	854.58	Joback Method
cpg	718.95	J/mol×K	889.04	Joback Method
cpg	730.02	J/mol×K	923.49	Joback Method
cpg	740.18	J/mol×K	957.94	Joback Method
cpg	749.43	J/mol×K	992.39	Joback Method
cpg	757.80	J/mol×K	1026.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377061&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