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

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

InchiKey: VZJZVSHTUAAANN-UHFFFAOYSA-N

Formula: C17H22BrFO4

SMILES: CCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 389.26

Physical Properties

Property code	Value	Unit	Source
gf	-462.92	kJ/mol	Joback Method
hf	-840.00	kJ/mol	Joback Method
hfus	46.99	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.535		Crippen Method
mcvol	260.780	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
rinpol	2409.00		NIST Webbook
rinpol	2409.00		NIST Webbook
tb	843.01	K	Joback Method
tc	1049.28	K	Joback Method
tf	537.52	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.34	J/mol×K	843.01	Joback Method
cpg	763.60	J/mol×K	877.39	Joback Method
cpg	775.86	J/mol×K	911.77	Joback Method
cpg	787.16	J/mol×K	946.14	Joback Method
cpg	797.50	J/mol×K	980.52	Joback Method
cpg	806.91	J/mol×K	1014.90	Joback Method
cpg	815.41	J/mol×K	1049.28	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=U377063&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