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

Inchi: InChI=1S/C14H16BrFO4/c1-2-19-13(17)4-3-5-14(18)20-9-10-8-11(16)6-7-12(10)15/h6-8

InchiKey: PZHWRTHGTKHXSG-UHFFFAOYSA-N

Formula: C14H16BrFO4

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

Mol. weight [g/mol]: 347.18

Physical Properties

Property code	Value	Unit	Source
gf	-488.18	kJ/mol	Joback Method
hf	-778.08	kJ/mol	Joback Method
hfus	39.22	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.365		Crippen Method
mcvol	218.510	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
tb	774.37	K	Joback Method
tc	983.85	K	Joback Method
tf	503.71	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.14	J/mol×K	774.37	Joback Method
cpg	596.40	J/mol×K	809.28	Joback Method
cpg	607.77	J/mol×K	844.20	Joback Method
cpg	618.29	J/mol×K	879.11	Joback Method
cpg	627.95	J/mol×K	914.02	Joback Method
cpg	636.77	J/mol×K	948.93	Joback Method
cpg	644.76	J/mol×K	983.85	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=U377062&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