Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C14H13BrF4O4/c1-8(14(17,18)19)22-12(20)3-2-4-13(21)23-11-6-5-9(16)7-10(1

InchiKey: JAQSBRFFGSCRFN-UHFFFAOYSA-N

Formula: C14H13BrF4O4

SMILES: CC(OC(=O)CCCC(=O)Oc1ccc(F)cc1Br)C(F)(F)F

Mol. weight [g/mol]: 401.15

Physical Properties

Property code	Value	Unit	Source
gf	-1072.21	kJ/mol	Joback Method
hf	-1380.44	kJ/mol	Joback Method
hfus	37.52	kJ/mol	Joback Method
hvap	70.15	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.158		Crippen Method
mcvol	223.820	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1845.00		NIST Webbook
rinpol	1845.00		NIST Webbook
tb	768.51	K	Joback Method
tc	968.93	K	Joback Method
tf	492.90	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.16	J/mol×K	768.51	Joback Method
cpg	621.31	J/mol×K	801.91	Joback Method
cpg	631.63	J/mol×K	835.32	Joback Method
cpg	641.15	J/mol×K	868.72	Joback Method
cpg	649.91	J/mol×K	902.12	Joback Method
cpg	657.92	J/mol×K	935.53	Joback Method
cpg	665.22	J/mol×K	968.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391821&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