Glutaric acid, 3-methylbut-2-en-1-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C16H18BrFO4/c1-11(2)8-9-21-15(19)4-3-5-16(20)22-14-7-6-12(18)10-13(14)1

InchiKey: YMQXMHYWPYOANT-UHFFFAOYSA-N

Formula: C16H18BrFO4

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

Mol. weight [g/mol]: 373.21

Physical Properties

Property code	Value	Unit	Source
gf	-399.67	kJ/mol	Joback Method
hf	-711.93	kJ/mol	Joback Method
hfus	43.29	kJ/mol	Joback Method
hvap	78.78	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.173		Crippen Method
mcvol	242.390	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
tb	824.17	K	Joback Method
tc	1038.63	K	Joback Method
tf	507.21	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.15	J/mol×K	824.17	Joback Method
cpg	679.73	J/mol×K	859.91	Joback Method
cpg	691.40	J/mol×K	895.66	Joback Method
cpg	702.18	J/mol×K	931.40	Joback Method
cpg	712.10	J/mol×K	967.14	Joback Method
cpg	721.21	J/mol×K	1002.88	Joback Method
cpg	729.53	J/mol×K	1038.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391827&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