Glutaric acid, 1-(2,6-difluorophenyl)ethyl isobutyl ester

Inchi: InChI=1S/C17H22F2O4/c1-11(2)10-22-15(20)8-5-9-16(21)23-12(3)17-13(18)6-4-7-14(17

InchiKey: YLWWQUFIBITGEA-UHFFFAOYSA-N

Formula: C17H22F2O4

SMILES: CC(C)COC(=O)CCCC(=O)OC(C)c1c(F)cccc1F

Mol. weight [g/mol]: 328.35

Physical Properties

Property code	Value	Unit	Source
gf	-676.93	kJ/mol	Joback Method
hf	-1073.00	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	72.94	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.939		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	775.24	K	Joback Method
tc	969.96	K	Joback Method
tf	448.31	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.94	J/mol×K	775.24	Joback Method
cpg	734.60	J/mol×K	807.69	Joback Method
cpg	748.30	J/mol×K	840.15	Joback Method
cpg	761.04	J/mol×K	872.60	Joback Method
cpg	772.84	J/mol×K	905.05	Joback Method
cpg	783.70	J/mol×K	937.51	Joback Method
cpg	793.64	J/mol×K	969.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377249&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

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