Glutaric acid, isobutyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C16H18F4O4/c1-9(2)7-23-12(21)4-3-5-13(22)24-8-10-6-11(17)15(19)16(20)14

InchiKey: GKRCBIDXBYKCKH-UHFFFAOYSA-N

Formula: C16H18F4O4

SMILES: CC(C)COC(=O)CCCC(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1091.79	kJ/mol	Joback Method
hf	-1462.24	kJ/mol	Joback Method
hfus	44.05	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.656		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	761.30	K	Joback Method
tc	945.98	K	Joback Method
tf	478.26	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.28	J/mol×K	761.30	Joback Method
cpg	690.37	J/mol×K	792.08	Joback Method
cpg	702.67	J/mol×K	822.86	Joback Method
cpg	714.17	J/mol×K	853.64	Joback Method
cpg	724.88	J/mol×K	884.42	Joback Method
cpg	734.79	J/mol×K	915.20	Joback Method
cpg	743.90	J/mol×K	945.98	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=U377440&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