Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C16H19F3O6/c1-10(16(17,18)19)24-13(20)8-5-9-14(21)25-15-11(22-2)6-4-7-1

InchiKey: ZDJKJERKSPVZQE-UHFFFAOYSA-N

Formula: C16H19F3O6

SMILES: COc1cccc(OC)c1OC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 364.31

Physical Properties

Property code	Value	Unit	Source
gf	-1084.88	kJ/mol	Joback Method
hf	-1516.38	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	73.81	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.273		Crippen Method
mcvol	244.470	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	2018.00		NIST Webbook
rinpol	2018.00		NIST Webbook
tb	793.68	K	Joback Method
tc	988.08	K	Joback Method
tf	499.51	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.23	J/mol×K	793.68	Joback Method
cpg	741.44	J/mol×K	826.08	Joback Method
cpg	753.66	J/mol×K	858.48	Joback Method
cpg	764.89	J/mol×K	890.88	Joback Method
cpg	775.12	J/mol×K	923.28	Joback Method
cpg	784.38	J/mol×K	955.68	Joback Method
cpg	792.64	J/mol×K	988.08	Joback Method

Sources

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=U391995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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