Glutaric acid, 2,2,3,3-tetrafluoropropyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C16H18F4O6/c1-23-10-5-3-6-11(24-2)14(10)26-13(22)8-4-7-12(21)25-9-16(19

InchiKey: SNAJIWKCFSOHSA-UHFFFAOYSA-N

Formula: C16H18F4O6

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

Mol. weight [g/mol]: 382.30

Physical Properties

Property code	Value	Unit	Source
gf	-1279.69	kJ/mol	Joback Method
hf	-1712.49	kJ/mol	Joback Method
hfus	39.79	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.223		Crippen Method
mcvol	246.240	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
tb	792.95	K	Joback Method
tc	982.95	K	Joback Method
tf	500.10	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.84	J/mol×K	792.95	Joback Method
cpg	748.66	J/mol×K	824.62	Joback Method
cpg	760.53	J/mol×K	856.28	Joback Method
cpg	771.45	J/mol×K	887.95	Joback Method
cpg	781.43	J/mol×K	919.62	Joback Method
cpg	790.45	J/mol×K	951.28	Joback Method
cpg	798.54	J/mol×K	982.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391996&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