Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C17H21F3O5/c1-11(2)23-13-7-4-5-8-14(13)25-16(22)10-6-9-15(21)24-12(3)17

InchiKey: HKNXHMUKCXMFSU-UHFFFAOYSA-N

Formula: C17H21F3O5

SMILES: CC(C)Oc1ccccc1OC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 362.34

Physical Properties

Property code	Value	Unit	Source
gf	-964.27	kJ/mol	Joback Method
hf	-1398.61	kJ/mol	Joback Method
hfus	34.98	kJ/mol	Joback Method
hvap	72.57	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.044		Crippen Method
mcvol	252.690	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook
tb	788.72	K	Joback Method
tc	983.81	K	Joback Method
tf	461.03	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.20	J/mol×K	788.72	Joback Method
cpg	772.30	J/mol×K	821.23	Joback Method
cpg	785.38	J/mol×K	853.75	Joback Method
cpg	797.46	J/mol×K	886.26	Joback Method
cpg	808.55	J/mol×K	918.78	Joback Method
cpg	818.68	J/mol×K	951.29	Joback Method
cpg	827.87	J/mol×K	983.81	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=U391863&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