Glutaric acid, pentyl 1-phenyl-2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C18H23F3O4/c1-2-3-7-13-24-15(22)11-8-12-16(23)25-17(18(19,20)21)14-9-5-

InchiKey: METURVVGIMGXJR-UHFFFAOYSA-N

Formula: C18H23F3O4

SMILES: CCCCCOC(=O)CCCC(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-838.78	kJ/mol	Joback Method
hf	-1270.28	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	72.11	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.737		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	2076.00		NIST Webbook
tb	784.64	K	Joback Method
tc	976.37	K	Joback Method
tf	452.55	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.85	J/mol×K	784.64	Joback Method
cpg	801.54	J/mol×K	816.60	Joback Method
cpg	815.23	J/mol×K	848.55	Joback Method
cpg	827.96	J/mol×K	880.51	Joback Method
cpg	839.77	J/mol×K	912.46	Joback Method
cpg	850.70	J/mol×K	944.42	Joback Method
cpg	860.77	J/mol×K	976.37	Joback Method

Sources

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=U377366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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