Glutaric acid, di(1-phenyl-2,2,2-trifluoroethyl) ester

Inchi: InChI=1S/C21H18F6O4/c22-20(23,24)18(14-8-3-1-4-9-14)30-16(28)12-7-13-17(29)31-19

InchiKey: FWOJYBOWTLUQGV-UHFFFAOYSA-N

Formula: C21H18F6O4

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

Mol. weight [g/mol]: 448.36

Physical Properties

Property code	Value	Unit	Source
gf	-1285.14	kJ/mol	Joback Method
hf	-1698.03	kJ/mol	Joback Method
hfus	40.41	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.850		Crippen Method
mcvol	284.730	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook
tb	874.10	K	Joback Method
tc	1081.55	K	Joback Method
tf	501.97	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.12	J/mol×K	874.10	Joback Method
cpg	899.47	J/mol×K	908.67	Joback Method
cpg	910.75	J/mol×K	943.25	Joback Method
cpg	921.04	J/mol×K	977.82	Joback Method
cpg	930.43	J/mol×K	1012.40	Joback Method
cpg	939.01	J/mol×K	1046.97	Joback Method
cpg	946.85	J/mol×K	1081.55	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=U377381&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