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

Inchi: InChI=1S/C17H21F3O4/c1-12(2)11-23-14(21)9-6-10-15(22)24-16(17(18,19)20)13-7-4-3-

InchiKey: QHMPUGJSGBEDQH-UHFFFAOYSA-N

Formula: C17H21F3O4

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

Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-849.64	kJ/mol	Joback Method
hf	-1254.92	kJ/mol	Joback Method
hfus	34.18	kJ/mol	Joback Method
hvap	69.50	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.203		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	1929.00		NIST Webbook
tb	761.32	K	Joback Method
tc	955.32	K	Joback Method
tf	426.28	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.09	J/mol×K	761.32	Joback Method
cpg	745.67	J/mol×K	793.65	Joback Method
cpg	759.26	J/mol×K	825.99	Joback Method
cpg	771.87	J/mol×K	858.32	Joback Method
cpg	783.56	J/mol×K	890.65	Joback Method
cpg	794.34	J/mol×K	922.99	Joback Method
cpg	804.27	J/mol×K	955.32	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=U377364&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