Glutaric acid, 2-methylhex-3-yl 1-phenyl-2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C20H27F3O4/c1-4-9-16(14(2)3)26-17(24)12-8-13-18(25)27-19(20(21,22)23)15

InchiKey: NSLJNSPKYXPQJU-UHFFFAOYSA-N

Formula: C20H27F3O4

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

Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-826.82	kJ/mol	Joback Method
hf	-1322.12	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	75.79	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.371		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	2136.00		NIST Webbook
tb	829.52	K	Joback Method
tc	1026.11	K	Joback Method
tf	445.09	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.19	J/mol×K	829.52	Joback Method
cpg	918.64	J/mol×K	862.28	Joback Method
cpg	932.99	J/mol×K	895.05	Joback Method
cpg	946.26	J/mol×K	927.81	Joback Method
cpg	958.51	J/mol×K	960.58	Joback Method
cpg	969.78	J/mol×K	993.34	Joback Method
cpg	980.12	J/mol×K	1026.11	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=U377367&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