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

Inchi: InChI=1S/C21H29F3O4/c1-2-3-4-5-6-10-16-27-18(25)14-11-15-19(26)28-20(21(22,23)24

InchiKey: WODPYFGQPUGXNU-UHFFFAOYSA-N

Formula: C21H29F3O4

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

Mol. weight [g/mol]: 402.45

Physical Properties

Property code	Value	Unit	Source
gf	-813.52	kJ/mol	Joback Method
hf	-1332.20	kJ/mol	Joback Method
hfus	48.06	kJ/mol	Joback Method
hvap	78.79	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.907		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2378.00		NIST Webbook
tb	853.28	K	Joback Method
tc	1048.99	K	Joback Method
tf	486.36	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.99	J/mol×K	853.28	Joback Method
cpg	976.51	J/mol×K	885.90	Joback Method
cpg	990.94	J/mol×K	918.52	Joback Method
cpg	1004.31	J/mol×K	951.13	Joback Method
cpg	1016.67	J/mol×K	983.75	Joback Method
cpg	1028.08	J/mol×K	1016.37	Joback Method
cpg	1038.57	J/mol×K	1048.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377370&Units=SI
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

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