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

Inchi: InChI=1S/C23H33F3O4/c1-2-3-4-5-6-7-8-12-18-29-20(27)16-13-17-21(28)30-22(23(24,2

InchiKey: NMLJGRQGAFJIAJ-UHFFFAOYSA-N

Formula: C23H33F3O4

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

Mol. weight [g/mol]: 430.50

Physical Properties

Property code	Value	Unit	Source
gf	-796.68	kJ/mol	Joback Method
hf	-1373.48	kJ/mol	Joback Method
hfus	53.24	kJ/mol	Joback Method
hvap	83.24	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.687		Crippen Method
mcvol	331.360	ml/mol	McGowan Method
pc	1033.24	kPa	Joback Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		NIST Webbook
tb	899.04	K	Joback Method
tc	1101.23	K	Joback Method
tf	508.90	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1080.81	J/mol×K	899.04	Joback Method
cpg	1096.96	J/mol×K	932.74	Joback Method
cpg	1111.90	J/mol×K	966.44	Joback Method
cpg	1125.71	J/mol×K	1000.14	Joback Method
cpg	1138.42	J/mol×K	1033.84	Joback Method
cpg	1150.12	J/mol×K	1067.53	Joback Method
cpg	1160.84	J/mol×K	1101.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377372&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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