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

Inchi: InChI=1S/C20H27F3O4/c1-2-3-4-5-9-15-26-17(24)13-10-14-18(25)27-19(20(21,22)23)16

InchiKey: LAHQSWYEFUKXBW-UHFFFAOYSA-N

Formula: C20H27F3O4

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

Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-821.94	kJ/mol	Joback Method
hf	-1311.56	kJ/mol	Joback Method
hfus	45.47	kJ/mol	Joback Method
hvap	76.57	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.517		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	830.40	K	Joback Method
tc	1024.08	K	Joback Method
tf	475.09	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.14	J/mol×K	830.40	Joback Method
cpg	917.38	J/mol×K	862.68	Joback Method
cpg	931.56	J/mol×K	894.96	Joback Method
cpg	944.72	J/mol×K	927.24	Joback Method
cpg	956.91	J/mol×K	959.52	Joback Method
cpg	968.16	J/mol×K	991.80	Joback Method
cpg	978.53	J/mol×K	1024.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377369&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