Glutaric acid, 1,1,1-trifluoroprop-2-yl 3-phenylpropyl ester

Inchi: InChI=1S/C17H21F3O4/c1-13(17(18,19)20)24-16(22)11-5-10-15(21)23-12-6-9-14-7-3-2-

InchiKey: SNRUEARCIYJOJV-UHFFFAOYSA-N

Formula: C17H21F3O4

SMILES: CC(OC(=O)CCCC(=O)OCCCc1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-847.20	kJ/mol	Joback Method
hf	-1249.64	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	69.89	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.827		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	761.76	K	Joback Method
tc	953.47	K	Joback Method
tf	441.28	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.54	J/mol×K	761.76	Joback Method
cpg	744.95	J/mol×K	793.71	Joback Method
cpg	758.38	J/mol×K	825.66	Joback Method
cpg	770.88	J/mol×K	857.62	Joback Method
cpg	782.48	J/mol×K	889.57	Joback Method
cpg	793.21	J/mol×K	921.52	Joback Method
cpg	803.11	J/mol×K	953.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391768&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