Glutaric acid, 1,1,1-trifluoroprop-2-yl phenethyl ester

Inchi: InChI=1S/C16H19F3O4/c1-12(16(17,18)19)23-15(21)9-5-8-14(20)22-11-10-13-6-3-2-4-7

InchiKey: PZSTVKKKTSWJAT-UHFFFAOYSA-N

Formula: C16H19F3O4

SMILES: CC(OC(=O)CCCC(=O)OCCc1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-855.62	kJ/mol	Joback Method
hf	-1229.00	kJ/mol	Joback Method
hfus	35.11	kJ/mol	Joback Method
hvap	67.66	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.437		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	738.88	K	Joback Method
tc	931.14	K	Joback Method
tf	430.01	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.23	J/mol×K	738.88	Joback Method
cpg	689.33	J/mol×K	770.92	Joback Method
cpg	702.48	J/mol×K	802.97	Joback Method
cpg	714.72	J/mol×K	835.01	Joback Method
cpg	726.08	J/mol×K	867.06	Joback Method
cpg	736.59	J/mol×K	899.10	Joback Method
cpg	746.28	J/mol×K	931.14	Joback Method

Sources

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=U391783&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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