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

Inchi: InChI=1S/C21H21F3O4/c1-15(21(22,23)24)27-18(25)13-8-14-19(26)28-20(16-9-4-2-5-10

InchiKey: MILBYQCYYWLDIQ-UHFFFAOYSA-N

Formula: C21H21F3O4

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

Mol. weight [g/mol]: 394.38

Physical Properties

Property code	Value	Unit	Source
gf	-703.55	kJ/mol	Joback Method
hf	-1100.95	kJ/mol	Joback Method
hfus	38.58	kJ/mol	Joback Method
hvap	80.68	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.984		Crippen Method
mcvol	279.420	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	879.52	K	Joback Method
tc	1095.68	K	Joback Method
tf	497.78	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.17	J/mol×K	879.52	Joback Method
cpg	877.60	J/mol×K	915.55	Joback Method
cpg	889.82	J/mol×K	951.57	Joback Method
cpg	900.91	J/mol×K	987.60	Joback Method
cpg	910.94	J/mol×K	1023.63	Joback Method
cpg	919.98	J/mol×K	1059.65	Joback Method
cpg	928.10	J/mol×K	1095.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393336&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

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