Glutaric acid, 2,2,3,3-tetrafluoropropyl diphenylmethyl ester

Inchi: InChI=1S/C21H20F4O4/c22-20(23)21(24,25)14-28-17(26)12-7-13-18(27)29-19(15-8-3-1-
InchiKey: LKKLVLGEAOUGNK-UHFFFAOYSA-N
Formula: C21H20F4O4
SMILES: O=C(CCCC(=O)OC(c1ccccc1)c1ccccc1)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 412.37

Physical Properties

Property code	Value	Unit	Source
gf	-898.36	kJ/mol	Joback Method
hf	-1297.06	kJ/mol	Joback Method
hfus	41.66	kJ/mol	Joback Method
hvap	79.86	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.933		Crippen Method
mcvol	281.190	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
tb	878.79	K	Joback Method
tc	1089.99	K	Joback Method
tf	498.37	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.47	J/mol×K	878.79	Joback Method
cpg	884.48	J/mol×K	913.99	Joback Method
cpg	896.34	J/mol×K	949.19	Joback Method
cpg	907.11	J/mol×K	984.39	Joback Method
cpg	916.86	J/mol×K	1019.59	Joback Method
cpg	925.66	J/mol×K	1054.79	Joback Method
cpg	933.57	J/mol×K	1089.99	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=U393337&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