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

Inchi: InChI=1S/C17H20F4O5/c1-11(2)25-12-6-3-4-7-13(12)26-15(23)9-5-8-14(22)24-10-17(20
InchiKey: ZZBVAUZBLLYESI-UHFFFAOYSA-N
Formula: C17H20F4O5
SMILES: CC(C)Oc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 380.33

Physical Properties

Property code	Value	Unit	Source
gf	-1159.08	kJ/mol	Joback Method
hf	-1594.72	kJ/mol	Joback Method
hfus	38.06	kJ/mol	Joback Method
hvap	71.76	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.993		Crippen Method
mcvol	254.460	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	787.99	K	Joback Method
tc	978.44	K	Joback Method
tf	461.62	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.80	J/mol×K	787.99	Joback Method
cpg	779.49	J/mol×K	819.73	Joback Method
cpg	792.19	J/mol×K	851.47	Joback Method
cpg	803.93	J/mol×K	883.21	Joback Method
cpg	814.73	J/mol×K	914.95	Joback Method
cpg	824.60	J/mol×K	946.69	Joback Method
cpg	833.58	J/mol×K	978.44	Joback Method

Sources

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=U391864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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