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

Inchi: InChI=1S/C17H20F4O4/c1-11(2)12-6-3-4-7-13(12)25-15(23)9-5-8-14(22)24-10-17(20,21
InchiKey: VDGUXUVUZSFFGQ-UHFFFAOYSA-N
Formula: C17H20F4O4
SMILES: CC(C)c1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1054.08	kJ/mol	Joback Method
hf	-1462.50	kJ/mol	Joback Method
hfus	36.87	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.329		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	765.57	K	Joback Method
tc	955.20	K	Joback Method
tf	439.39	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.96	J/mol×K	765.57	Joback Method
cpg	751.97	J/mol×K	797.17	Joback Method
cpg	765.04	J/mol×K	828.78	Joback Method
cpg	777.19	J/mol×K	860.38	Joback Method
cpg	788.45	J/mol×K	891.99	Joback Method
cpg	798.86	J/mol×K	923.59	Joback Method
cpg	808.45	J/mol×K	955.20	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=U391910&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

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