Glutaric acid, ethyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C14H14F4O4/c1-2-21-10(19)4-3-5-11(20)22-7-8-6-9(15)13(17)14(18)12(8)16/h

InchiKey: JCEBITXHDMKHKW-UHFFFAOYSA-N

Formula: C14H14F4O4

SMILES: CCOC(=O)CCCC(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 322.25

Physical Properties

Property code	Value	Unit	Source
gf	-1106.19	kJ/mol	Joback Method
hf	-1415.68	kJ/mol	Joback Method
hfus	42.39	kJ/mol	Joback Method
hvap	66.73	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.020		Crippen Method
mcvol	206.320	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	715.98	K	Joback Method
tc	898.17	K	Joback Method
tf	470.72	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.63	J/mol×K	715.98	Joback Method
cpg	580.60	J/mol×K	746.35	Joback Method
cpg	591.91	J/mol×K	776.71	Joback Method
cpg	602.55	J/mol×K	807.08	Joback Method
cpg	612.51	J/mol×K	837.44	Joback Method
cpg	621.80	J/mol×K	867.81	Joback Method
cpg	630.40	J/mol×K	898.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377438&Units=SI

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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