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

Inchi: InChI=1S/C15H16F4O4/c1-10-4-2-5-11(8-10)23-13(21)7-3-6-12(20)22-9-15(18,19)14(16

InchiKey: UYMGINXTWOUSGS-UHFFFAOYSA-N

Formula: C15H16F4O4

SMILES: Cc1cccc(OC(=O)CCCC(=O)OCC(F)(F)C(F)F)c1

Mol. weight [g/mol]: 336.28

Physical Properties

Property code	Value	Unit	Source
gf	-1068.48	kJ/mol	Joback Method
hf	-1415.94	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	65.28	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.514		Crippen Method
mcvol	220.410	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
tb	720.25	K	Joback Method
tc	908.26	K	Joback Method
tf	431.85	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.94	J/mol×K	720.25	Joback Method
cpg	641.07	J/mol×K	751.59	Joback Method
cpg	653.35	J/mol×K	782.92	Joback Method
cpg	664.80	J/mol×K	814.26	Joback Method
cpg	675.44	J/mol×K	845.59	Joback Method
cpg	685.30	J/mol×K	876.93	Joback Method
cpg	694.41	J/mol×K	908.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391947&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