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

Inchi: InChI=1S/C14H13F5O4/c15-9-3-1-4-10(7-9)23-12(21)6-2-5-11(20)22-8-14(18,19)13(16)1

InchiKey: RMBNSIFXQVIZAD-UHFFFAOYSA-N

Formula: C14H13F5O4

SMILES: O=C(CCCC(=O)Oc1cccc(F)c1)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 340.24

Physical Properties

Property code	Value	Unit	Source
gf	-1271.71	kJ/mol	Joback Method
hf	-1591.41	kJ/mol	Joback Method
hfus	35.70	kJ/mol	Joback Method
hvap	62.24	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.345		Crippen Method
mcvol	208.090	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1734.00		NIST Webbook
tb	696.64	K	Joback Method
tc	879.53	K	Joback Method
tf	421.17	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.80	J/mol×K	696.64	Joback Method
cpg	595.05	J/mol×K	727.12	Joback Method
cpg	606.52	J/mol×K	757.60	Joback Method
cpg	617.22	J/mol×K	788.08	Joback Method
cpg	627.19	J/mol×K	818.56	Joback Method
cpg	636.44	J/mol×K	849.05	Joback Method
cpg	645.00	J/mol×K	879.53	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=U392084&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