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

Inchi: InChI=1S/C14H12F6O4/c15-9-4-1-2-5-10(9)24-12(22)7-3-6-11(21)23-8-13(16,17)14(18,1

InchiKey: RIFVJWDRMSESDA-UHFFFAOYSA-N

Formula: C14H12F6O4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 358.23

Physical Properties

Property code	Value	Unit	Source
gf	-1461.24	kJ/mol	Joback Method
hf	-1790.99	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.642		Crippen Method
mcvol	209.860	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
tb	693.12	K	Joback Method
tc	874.60	K	Joback Method
tf	439.18	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.01	J/mol×K	693.12	Joback Method
cpg	604.87	J/mol×K	723.37	Joback Method
cpg	615.93	J/mol×K	753.61	Joback Method
cpg	626.22	J/mol×K	783.86	Joback Method
cpg	635.77	J/mol×K	814.11	Joback Method
cpg	644.63	J/mol×K	844.35	Joback Method
cpg	652.82	J/mol×K	874.60	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=U393672&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