Glutaric acid, 2,2,3,3-tetrafluoropropyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C14H11F7O4/c15-7-4-5-8(12(17)11(7)16)25-10(23)3-1-2-9(22)24-6-14(20,21)1

InchiKey: CDXHSMWZSDYIHJ-UHFFFAOYSA-N

Formula: C14H11F7O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)c(F)c1F)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 376.22

Physical Properties

Property code	Value	Unit	Source
gf	-1680.59	kJ/mol	Joback Method
hf	-2006.57	kJ/mol	Joback Method
hfus	41.09	kJ/mol	Joback Method
hvap	61.93	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.623		Crippen Method
mcvol	211.630	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
tb	705.14	K	Joback Method
tc	879.55	K	Joback Method
tf	447.39	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.63	J/mol×K	705.14	Joback Method
cpg	607.84	J/mol×K	734.21	Joback Method
cpg	618.37	J/mol×K	763.28	Joback Method
cpg	628.24	J/mol×K	792.35	Joback Method
cpg	637.45	J/mol×K	821.42	Joback Method
cpg	646.02	J/mol×K	850.48	Joback Method
cpg	653.97	J/mol×K	879.55	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=U393633&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