Glutaric acid, 3,5-difluorophenyl propyl ester

Inchi: InChI=1S/C14H16F2O4/c1-2-6-19-13(17)4-3-5-14(18)20-12-8-10(15)7-11(16)9-12/h7-9H
InchiKey: QOYRRPLSBFHGQM-UHFFFAOYSA-N
Formula: C14H16F2O4
SMILES: CCCOC(=O)CCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 286.27

Physical Properties

Property code	Value	Unit	Source
gf	-697.31	kJ/mol	Joback Method
hf	-1000.52	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	67.04	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.994		Crippen Method
mcvol	202.780	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook
tb	707.48	K	Joback Method
tc	899.73	K	Joback Method
tf	444.50	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.85	J/mol×K	707.48	Joback Method
cpg	567.96	J/mol×K	739.52	Joback Method
cpg	580.30	J/mol×K	771.56	Joback Method
cpg	591.88	J/mol×K	803.61	Joback Method
cpg	602.68	J/mol×K	835.65	Joback Method
cpg	612.73	J/mol×K	867.69	Joback Method
cpg	622.01	J/mol×K	899.73	Joback Method

Sources

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=U358626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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