Glutaric acid, 3,5-difluorophenyl isohexyl ester

Inchi: InChI=1S/C17H22F2O4/c1-12(2)5-4-8-22-16(20)6-3-7-17(21)23-15-10-13(18)9-14(19)11
InchiKey: MTHUBQXXWJQNLU-UHFFFAOYSA-N
Formula: C17H22F2O4
SMILES: CC(C)CCCOC(=O)CCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 328.35

Physical Properties

Property code	Value	Unit	Source
gf	-674.49	kJ/mol	Joback Method
hf	-1067.72	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.020		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	775.68	K	Joback Method
tc	968.23	K	Joback Method
tf	463.31	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.39	J/mol×K	775.68	Joback Method
cpg	733.89	J/mol×K	807.77	Joback Method
cpg	747.45	J/mol×K	839.86	Joback Method
cpg	760.09	J/mol×K	871.96	Joback Method
cpg	771.81	J/mol×K	904.05	Joback Method
cpg	782.62	J/mol×K	936.14	Joback Method
cpg	792.54	J/mol×K	968.23	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=U358630&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