Glutaric acid, di(3,5-difluorophenyl) ester

Inchi: InChI=1S/C17H12F4O4/c18-10-4-11(19)7-14(6-10)24-16(22)2-1-3-17(23)25-15-8-12(20)5-13(21)9-15/h4-9H,1-3H2

InchiKey: FQLRVTBKUWPDHF-UHFFFAOYSA-N

Formula: C17H12F4O4

SMILES: O=C(CCCC(=O)Oc1cc(F)cc(F)c1)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 356.27

Physical Properties

Property code	Value	Unit	Source
gf	-968.52	kJ/mol	Joback Method
hf	-1241.07	kJ/mol	Joback Method
hfus	44.21	kJ/mol	Joback Method
hvap	75.68	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.924		Crippen Method
mcvol	224.830	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	811.30	K	Joback Method
tc	1016.55	K	Joback Method
tf	530.95	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.26	J/mol×K	811.30	Joback Method
cpg	650.67	J/mol×K	845.51	Joback Method
cpg	661.13	J/mol×K	879.72	Joback Method
cpg	670.65	J/mol×K	913.92	Joback Method
cpg	679.23	J/mol×K	948.13	Joback Method
cpg	686.89	J/mol×K	982.34	Joback Method
cpg	693.63	J/mol×K	1016.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358643&Units=SI
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

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