Glutaric acid, di(2-fluoro-3-trifluoromethylphenyl) ester

Inchi: InChI=1S/C19H12F8O4/c20-16-10(18(22,23)24)4-1-6-12(16)30-14(28)8-3-9-15(29)31-13

InchiKey: ULWSLEUPGJJKNK-UHFFFAOYSA-N

Formula: C19H12F8O4

SMILES: O=C(CCCC(=O)Oc1cccc(C(F)(F)F)c1F)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 456.28

Physical Properties

Property code	Value	Unit	Source
gf	-1725.24	kJ/mol	Joback Method
hf	-2084.29	kJ/mol	Joback Method
hfus	46.88	kJ/mol	Joback Method
hvap	74.27	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.684		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	2194.00		NIST Webbook
rinpol	2194.00		NIST Webbook
tb	847.68	K	Joback Method
tc	1045.79	K	Joback Method
tf	560.69	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.83	J/mol×K	847.68	Joback Method
cpg	793.52	J/mol×K	880.70	Joback Method
cpg	803.29	J/mol×K	913.72	Joback Method
cpg	812.20	J/mol×K	946.73	Joback Method
cpg	820.30	J/mol×K	979.75	Joback Method
cpg	827.63	J/mol×K	1012.77	Joback Method
cpg	834.24	J/mol×K	1045.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393630&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