Glutaric acid, 2-methylpent-3-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C17H21F3O4/c1-4-12(10(2)3)23-14(21)6-5-7-15(22)24-13-9-8-11(18)16(19)17

InchiKey: BRSXFVKPKIOKKL-UHFFFAOYSA-N

Formula: C17H21F3O4

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

Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-881.37	kJ/mol	Joback Method
hf	-1280.58	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	72.78	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.157		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	779.49	K	Joback Method
tc	970.10	K	Joback Method
tf	461.42	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.75	J/mol×K	779.49	Joback Method
cpg	740.87	J/mol×K	811.26	Joback Method
cpg	754.08	J/mol×K	843.03	Joback Method
cpg	766.37	J/mol×K	874.80	Joback Method
cpg	777.76	J/mol×K	906.57	Joback Method
cpg	788.24	J/mol×K	938.33	Joback Method
cpg	797.84	J/mol×K	970.10	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=U393636&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