Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C16H19F3O4/c1-10-6-4-7-13(11(10)2)23-15(21)9-5-8-14(20)22-12(3)16(17,18

InchiKey: YMJGBUIJPFOVJP-UHFFFAOYSA-N

Formula: C16H19F3O4

SMILES: Cc1cccc(OC(=O)CCCC(=O)OC(C)C(F)(F)F)c1C

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-874.88	kJ/mol	Joback Method
hf	-1251.94	kJ/mol	Joback Method
hfus	34.34	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.873		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
tb	748.84	K	Joback Method
tc	942.76	K	Joback Method
tf	455.05	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.50	J/mol×K	748.84	Joback Method
cpg	687.38	J/mol×K	781.16	Joback Method
cpg	700.34	J/mol×K	813.48	Joback Method
cpg	712.41	J/mol×K	845.80	Joback Method
cpg	723.61	J/mol×K	878.12	Joback Method
cpg	733.96	J/mol×K	910.44	Joback Method
cpg	743.49	J/mol×K	942.76	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=U392211&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