Glutaric acid, ethyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C14H15F3O4/c1-2-20-12(18)4-3-5-13(19)21-8-9-10(15)6-7-11(16)14(9)17/h6-7

InchiKey: PSSPGRLFMPKTDF-UHFFFAOYSA-N

Formula: C14H15F3O4

SMILES: CCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F

Mol. weight [g/mol]: 304.26

Physical Properties

Property code	Value	Unit	Source
gf	-901.75	kJ/mol	Joback Method
hf	-1208.10	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.880		Crippen Method
mcvol	204.550	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	711.73	K	Joback Method
tc	898.61	K	Joback Method
tf	457.61	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.77	J/mol×K	711.73	Joback Method
cpg	574.28	J/mol×K	742.88	Joback Method
cpg	586.08	J/mol×K	774.02	Joback Method
cpg	597.16	J/mol×K	805.17	Joback Method
cpg	607.53	J/mol×K	836.32	Joback Method
cpg	617.18	J/mol×K	867.47	Joback Method
cpg	626.11	J/mol×K	898.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376893&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