Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-methylbutyl ester

Inchi: InChI=1S/C13H21F3O4/c1-4-9(2)8-19-11(17)6-5-7-12(18)20-10(3)13(14,15)16/h9-10H,4
InchiKey: OBBXIBFMPHJOIU-UHFFFAOYSA-N
Formula: C13H21F3O4
SMILES: CCC(C)COC(=O)CCCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 298.30

Physical Properties

Property code	Value	Unit	Source
gf	-995.73	kJ/mol	Joback Method
hf	-1408.89	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.240		Crippen Method
mcvol	214.220	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	1433.00		NIST Webbook
rinpol	1433.00		NIST Webbook
tb	643.12	K	Joback Method
tc	813.93	K	Joback Method
tf	354.78	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.03	J/mol×K	643.12	Joback Method
cpg	610.47	J/mol×K	671.59	Joback Method
cpg	624.20	J/mol×K	700.06	Joback Method
cpg	637.22	J/mol×K	728.53	Joback Method
cpg	649.55	J/mol×K	756.99	Joback Method
cpg	661.20	J/mol×K	785.46	Joback Method
cpg	672.20	J/mol×K	813.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391679&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