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

Inchi: InChI=1S/C14H23F3O4/c1-5-11(9(2)3)21-13(19)8-6-7-12(18)20-10(4)14(15,16)17/h9-11
InchiKey: HEZQSPKJCDXEQV-UHFFFAOYSA-N
Formula: C14H23F3O4
SMILES: CCC(OC(=O)CCCC(=O)OC(C)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 312.33

Physical Properties

Property code	Value	Unit	Source
gf	-989.75	kJ/mol	Joback Method
hf	-1434.81	kJ/mol	Joback Method
hfus	28.85	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.628		Crippen Method
mcvol	228.310	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	665.56	K	Joback Method
tc	838.45	K	Joback Method
tf	351.05	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.90	J/mol×K	665.56	Joback Method
cpg	665.04	J/mol×K	694.38	Joback Method
cpg	679.41	J/mol×K	723.19	Joback Method
cpg	693.01	J/mol×K	752.01	Joback Method
cpg	705.87	J/mol×K	780.82	Joback Method
cpg	717.99	J/mol×K	809.64	Joback Method
cpg	729.40	J/mol×K	838.45	Joback Method

Sources

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=U393489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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