Glutaric acid, 2,2,2-triluoroethyl isobutyl ester

Inchi: InChI=1S/C11H17F3O4/c1-8(2)6-17-9(15)4-3-5-10(16)18-7-11(12,13)14/h8H,3-7H2,1-2H
InchiKey: ZCWXOIKXEBLDII-UHFFFAOYSA-N
Formula: C11H17F3O4
SMILES: CC(C)COC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 270.25

Physical Properties

Property code	Value	Unit	Source
gf	-1010.13	kJ/mol	Joback Method
hf	-1362.33	kJ/mol	Joback Method
hfus	28.12	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.461		Crippen Method
mcvol	186.040	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	1267.00		NIST Webbook
rinpol	1267.00		NIST Webbook
tb	597.80	K	Joback Method
tc	767.15	K	Joback Method
tf	347.24	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.95	J/mol×K	597.80	Joback Method
cpg	506.03	J/mol×K	626.03	Joback Method
cpg	518.50	J/mol×K	654.25	Joback Method
cpg	530.35	J/mol×K	682.48	Joback Method
cpg	541.61	J/mol×K	710.70	Joback Method
cpg	552.28	J/mol×K	738.93	Joback Method
cpg	562.38	J/mol×K	767.15	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=U380509&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