Glutaric acid, 2,2,2-triluoroethyl propyl ester

Inchi: InChI=1S/C10H15F3O4/c1-2-6-16-8(14)4-3-5-9(15)17-7-10(11,12)13/h2-7H2,1H3
InchiKey: YCHZWCBSMYBBAV-UHFFFAOYSA-N
Formula: C10H15F3O4
SMILES: CCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 256.22

Physical Properties

Property code	Value	Unit	Source
gf	-1016.11	kJ/mol	Joback Method
hf	-1336.41	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.215		Crippen Method
mcvol	171.950	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	575.36	K	Joback Method
tc	742.77	K	Joback Method
tf	350.97	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.52	J/mol×K	575.36	Joback Method
cpg	455.70	J/mol×K	603.26	Joback Method
cpg	467.32	J/mol×K	631.16	Joback Method
cpg	478.40	J/mol×K	659.06	Joback Method
cpg	488.93	J/mol×K	686.96	Joback Method
cpg	498.94	J/mol×K	714.87	Joback Method
cpg	508.43	J/mol×K	742.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380508&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

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