Glutaric acid, ethyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C11H13F7O4/c1-2-21-7(19)4-3-5-8(20)22-6-9(12,13)10(14,15)11(16,17)18/h2-

InchiKey: IHPJOTUIIGZDDR-UHFFFAOYSA-N

Formula: C11H13F7O4

SMILES: CCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 342.21

Physical Properties

Property code	Value	Unit	Source
gf	-1781.25	kJ/mol	Joback Method
hf	-2158.99	kJ/mol	Joback Method
hfus	29.14	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.096		Crippen Method
mcvol	193.120	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	1352.00		NIST Webbook
tb	588.86	K	Joback Method
tc	746.26	K	Joback Method
tf	369.44	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.50	J/mol×K	588.86	Joback Method
cpg	543.48	J/mol×K	615.09	Joback Method
cpg	554.78	J/mol×K	641.33	Joback Method
cpg	565.44	J/mol×K	667.56	Joback Method
cpg	575.48	J/mol×K	693.79	Joback Method
cpg	584.92	J/mol×K	720.02	Joback Method
cpg	593.80	J/mol×K	746.26	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=U377545&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