Glutaric acid, 2,2,3,3-tetrafluoropropyl isobutyl ester

Inchi: InChI=1S/C12H18F4O4/c1-8(2)6-19-9(17)4-3-5-10(18)20-7-12(15,16)11(13)14/h8,11H,3

InchiKey: ANYSABBYQDBCRI-UHFFFAOYSA-N

Formula: C12H18F4O4

SMILES: CC(C)COC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 302.26

Physical Properties

Property code	Value	Unit	Source
gf	-1198.96	kJ/mol	Joback Method
hf	-1584.36	kJ/mol	Joback Method
hfus	30.27	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.799		Crippen Method
mcvol	201.900	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	619.51	K	Joback Method
tc	785.03	K	Joback Method
tf	344.10	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.03	J/mol×K	619.51	Joback Method
cpg	565.44	J/mol×K	647.10	Joback Method
cpg	578.21	J/mol×K	674.68	Joback Method
cpg	590.35	J/mol×K	702.27	Joback Method
cpg	601.86	J/mol×K	729.86	Joback Method
cpg	612.77	J/mol×K	757.45	Joback Method
cpg	623.07	J/mol×K	785.03	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=U391498&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