glutamic acid, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C13H20F3NO5/c1-7(2)21-10(18)6-5-9(11(19)22-8(3)4)17-12(20)13(14,15)16/h
InchiKey: YVPCHKAGOSZGIG-UHFFFAOYSA-N
Formula: C13H20F3NO5
SMILES: CC(C)OC(=O)CCC(NC(=O)C(F)(F)F)C(=O)OC(C)C
Mol. weight [g/mol]: 327.30

Physical Properties

Property code	Value	Unit	Source
gf	-1037.70	kJ/mol	Joback Method
hf	-1473.28	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	71.11	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	1.717		Crippen Method
mcvol	225.770	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	746.72	K	Joback Method
tc	931.16	K	Joback Method
tf	442.37	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.00	J/mol×K	746.72	Joback Method
cpg	684.98	J/mol×K	777.46	Joback Method
cpg	697.13	J/mol×K	808.20	Joback Method
cpg	708.47	J/mol×K	838.94	Joback Method
cpg	719.00	J/mol×K	869.68	Joback Method
cpg	728.76	J/mol×K	900.42	Joback Method
cpg	737.76	J/mol×K	931.16	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=R267873&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