isovaleryl glycine, PFP-TFE

Inchi: InChI=1S/C12H13F8NO4/c1-6(2)3-7(22)21(4-8(23)25-5-10(13,14)15)9(24)11(16,17)12(1
InchiKey: XVNQEEQASAPZSQ-UHFFFAOYSA-N
Formula: C12H13F8NO4
SMILES: CC(C)CC(=O)N(CC(=O)OCC(F)(F)F)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 387.22

Physical Properties

Property code	Value	Unit	Source
gf	-1883.22	kJ/mol	Joback Method
hf	-2293.85	kJ/mol	Joback Method
hfus	34.72	kJ/mol	Joback Method
hvap	56.19	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.691		Crippen Method
mcvol	214.660	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
tb	654.46	K	Joback Method
tc	816.77	K	Joback Method
tf	426.47	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.38	J/mol×K	654.46	Joback Method
cpg	632.94	J/mol×K	681.51	Joback Method
cpg	643.74	J/mol×K	708.56	Joback Method
cpg	653.84	J/mol×K	735.61	Joback Method
cpg	663.26	J/mol×K	762.66	Joback Method
cpg	672.05	J/mol×K	789.72	Joback Method
cpg	680.26	J/mol×K	816.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321709&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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