3-methylcrotonyl glycine, PFP-TFE

Inchi: InChI=1S/C12H11F8NO4/c1-6(2)3-7(22)21(4-8(23)25-5-10(13,14)15)9(24)11(16,17)12(1
InchiKey: IKVUIVMODUOYBG-UHFFFAOYSA-N
Formula: C12H11F8NO4
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]: 385.21

Physical Properties

Property code	Value	Unit	Source
gf	-1809.11	kJ/mol	Joback Method
hf	-2181.14	kJ/mol	Joback Method
hfus	37.13	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.611		Crippen Method
mcvol	210.360	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	1247.00		NIST Webbook
tb	658.94	K	Joback Method
tc	825.22	K	Joback Method
tf	422.43	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.61	J/mol×K	658.94	Joback Method
cpg	609.48	J/mol×K	686.65	Joback Method
cpg	619.59	J/mol×K	714.37	Joback Method
cpg	629.01	J/mol×K	742.08	Joback Method
cpg	637.77	J/mol×K	769.79	Joback Method
cpg	645.93	J/mol×K	797.51	Joback Method
cpg	653.54	J/mol×K	825.22	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=R321670&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