hexanoyl glycine, PFP-TFE

Inchi: InChI=1S/C13H15F8NO4/c1-2-3-4-5-8(23)22(6-9(24)26-7-11(14,15)16)10(25)12(17,18)1
InchiKey: HJCYPTXJAGTRKZ-UHFFFAOYSA-N
Formula: C13H15F8NO4
SMILES: CCCCCC(=O)N(CC(=O)OCC(F)(F)F)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 401.25

Physical Properties

Property code	Value	Unit	Source
gf	-1872.36	kJ/mol	Joback Method
hf	-2309.21	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	58.80	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.225		Crippen Method
mcvol	228.750	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	1293.00		NIST Webbook
tb	677.78	K	Joback Method
tc	839.75	K	Joback Method
tf	452.74	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.88	J/mol×K	677.78	Joback Method
cpg	684.74	J/mol×K	704.77	Joback Method
cpg	695.85	J/mol×K	731.77	Joback Method
cpg	706.24	J/mol×K	758.76	Joback Method
cpg	715.98	J/mol×K	785.76	Joback Method
cpg	725.08	J/mol×K	812.75	Joback Method
cpg	733.61	J/mol×K	839.75	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=R321690&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