octanoyl glycine, PFP-TFE

Inchi: InChI=1S/C15H19F8NO4/c1-2-3-4-5-6-7-10(25)24(8-11(26)28-9-13(16,17)18)12(27)14(1

InchiKey: QNTQAXCHJZLGLX-UHFFFAOYSA-N

Formula: C15H19F8NO4

SMILES: CCCCCCCC(=O)N(CC(=O)OCC(F)(F)F)C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 429.30

Physical Properties

Property code	Value	Unit	Source
gf	-1855.52	kJ/mol	Joback Method
hf	-2350.49	kJ/mol	Joback Method
hfus	46.01	kJ/mol	Joback Method
hvap	63.25	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.005		Crippen Method
mcvol	256.930	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
tb	723.54	K	Joback Method
tc	889.82	K	Joback Method
tf	475.28	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.25	J/mol×K	723.54	Joback Method
cpg	793.03	J/mol×K	751.25	Joback Method
cpg	805.00	J/mol×K	778.97	Joback Method
cpg	816.23	J/mol×K	806.68	Joback Method
cpg	826.76	J/mol×K	834.39	Joback Method
cpg	836.63	J/mol×K	862.10	Joback Method
cpg	845.90	J/mol×K	889.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321714&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