L-Glutamine, N,N'-di(trifluoroacetyl)-, 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C12H9F11N2O5/c13-9(14,12(21,22)23)3-30-6(27)4(24-7(28)10(15,16)17)1-2-5

InchiKey: LSKPLPZJWRMRRG-UHFFFAOYSA-N

Formula: C12H9F11N2O5

SMILES: O=C(OCC(F)(F)C(F)(F)F)C(CCC(O)=NC(=O)C(F)(F)F)N=C(O)C(F)(F)F

Mol. weight [g/mol]: 470.19

Physical Properties

Property code	Value	Unit	Source
hf	-3005.48	kJ/mol	Joback Method
hvap	83.80	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.440		Crippen Method
mcvol	231.520	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
tb	920.21	K	Joback Method
tc	1130.77	K	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=U352336&Units=SI

Legend

hf: Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature