L-Threonine, N,O-di(trifluoroacetyl)-, 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C11H8F11NO5/c1-3(28-7(26)10(17,18)19)4(23-6(25)9(14,15)16)5(24)27-2-8(1

InchiKey: MCRBGONFYZRMGW-UHFFFAOYSA-N

Formula: C11H8F11NO5

SMILES: CC(OC(=O)C(F)(F)F)C(NC(=O)C(F)(F)F)C(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 443.17

Physical Properties

Property code	Value	Unit	Source
gf	-2602.06	kJ/mol	Joback Method
hf	-3021.85	kJ/mol	Joback Method
hfus	33.70	kJ/mol	Joback Method
hvap	56.63	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.268		Crippen Method
mcvol	211.750	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	977.80		NIST Webbook
tb	685.87	K	Joback Method
tc	848.24	K	Joback Method
tf	446.81	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.82	J/mol×K	685.87	Joback Method
cpg	646.44	J/mol×K	712.93	Joback Method
cpg	655.35	J/mol×K	739.99	Joback Method
cpg	663.58	J/mol×K	767.06	Joback Method
cpg	671.18	J/mol×K	794.12	Joback Method
cpg	678.19	J/mol×K	821.18	Joback Method
cpg	684.64	J/mol×K	848.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352343&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