Creatinine, butyl ester, TFA

Inchi: InChI=1S/C12H15F6N3O4/c1-3-4-5-25-7(22)6-21(2)10(19-8(23)11(13,14)15)20-9(24)12(
InchiKey: PZWYKKVAQMROBZ-UHFFFAOYSA-N
Formula: C12H15F6N3O4
SMILES: CCCCOC(=O)CN(C)C(=NC(=O)C(F)(F)F)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 379.26

Physical Properties

Property code	Value	Unit	Source
hf	-1761.70	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.385		Crippen Method
mcvol	226.780	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	1440.00		NIST Webbook
tb	786.32	K	Joback Method
tc	971.13	K	Joback Method

Sources

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=R31971&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:
https://www.chemeo.com/cid/14-200-3/Creatinine-butyl-ester-TFA.pdf
Generated by Cheméo on 2024-04-19 18:25:44.553154782 +0000 UTC m=+15840393.473732097.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.