Ser TFA Bu

Other names: Ser TFA Bu
Inchi: InChI=1S/C9H14F3NO4/c1-2-3-4-17-7(15)6(5-14)13-8(16)9(10,11)12/h6,14H,2-5H2,1H3
InchiKey: YRBVCQWRGDWXAR-UHFFFAOYSA-N
Formula: C9H14F3NO4
SMILES: CCCCOC(=O)C(CO)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 257.21

Physical Properties

Property code	Value	Unit	Source
hf	-1449.21	kJ/mol	Cheméo Relay (1.0)
hfus	30.94	kJ/mol	Joback Method
hvap	77.63	kJ/mol	Cheméo Relay (1.0)
logp	0.369		Crippen Method
mcvol	167.840	ml/mol	McGowan Method
rinpol	1257.00		NIST Webbook
tb	519.56	K	Cheméo Relay (1.0)
tf	317.84	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.14	J/mol×K	671.97	Joback Method
cpg	484.14	J/mol×K	700.46	Joback Method
cpg	493.58	J/mol×K	728.95	Joback Method
cpg	502.48	J/mol×K	757.44	Joback Method
cpg	510.86	J/mol×K	785.93	Joback Method
cpg	518.74	J/mol×K	814.42	Joback Method
cpg	526.13	J/mol×K	842.91	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23403432&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point