

Ser, butyl ester, TFA

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
CAS:	23403-43-2

Physical Properties

Property code	Value	Unit	Source
gf	-969.40	kJ/mol	Joback Method
hf	-1287.59	kJ/mol	Joback Method
hfus	30.94	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	0.369		Crippen Method
mcvol	167.840	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1257.00		NIST Webbook
tb	671.97	K	Joback Method
tc	842.91	K	Joback Method
tf	415.95	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23403432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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