

L-Threonine, N-(trifluoroacetyl)-, butyl ester

Other names:	Threonine, N-(trifluoroacetyl)-, butyl ester, L-Threonine, N-(trifluoroacetyl)-, butyl ester Thr, butyl ester, TFA Thr, TFA, butyl ester Thr TFA Bu
Inchi:	InChI=1S/C10H16F3NO4/c1-3-4-5-18-8(16)7(6(2)15)14-9(17)10(11,12)13/h6-7,15H,3-5H
InchiKey:	FKTFFGPAZUBWBK-NKWVEPMBSA-N
Formula:	C10H16F3NO4
SMILES:	CCCCOC(=O)C(NC(=O)C(F)(F)F)C(C)O
Mol. weight [g/mol]:	271.23
CAS:	23403-41-0

Physical Properties

Property code	Value	Unit	Source
gf	-963.42	kJ/mol	Joback Method
hf	-1313.51	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	72.35	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	0.758		Crippen Method
mcvol	181.930	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1246.00		NIST Webbook
rinpol	1246.00		NIST Webbook
tb	694.41	K	Joback Method
tc	867.67	K	Joback Method
tf	412.22	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.60	J/mol×K	694.41	Joback Method
cpg	536.33	J/mol×K	723.29	Joback Method

cpg	546.46	J/mol×K	752.16	Joback Method
cpg	555.99	J/mol×K	781.04	Joback Method
cpg	564.94	J/mol×K	809.91	Joback Method
cpg	573.35	J/mol×K	838.79	Joback Method
cpg	581.22	J/mol×K	867.67	Joback Method

Sources

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=C23403410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

<https://www.chemeo.com/cid/41-076-2/L-Threonine-N-trifluoroacetyl-butyl-ester.pdf>

Generated by Cheméo on 2025-12-05 21:37:58.88354472 +0000 UTC m=+4718876.413585395.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.