

Glycine, n-(trifluoroacetyl)-, butyl ester

Other names:	Gly, butyl ester, TFA Gly TFA Bu
Inchi:	InChI=1S/C8H12F3NO3/c1-2-3-4-15-6(13)5-12-7(14)8(9,10)11/h2-5H2,1H3,(H,12,14)
InchiKey:	ZTNMNXKYGGHKLS-UHFFFAOYSA-N
Formula:	C8H12F3NO3
SMILES:	CCCCOC(=O)CNC(=O)C(F)(F)F
Mol. weight [g/mol]:	227.18

Physical Properties

Property code	Value	Unit	Source
af	0.5784		Cheméo Relay (1.0)
hf	-1249.70	kJ/mol	Cheméo Relay (1.0)
hfus	27.79	kJ/mol	Joback Method
hvap	60.56	kJ/mol	Cheméo Relay (1.0)
ie	10.15	eV	Cheméo Relay (1.0)
log10ws	-1.46		Cheméo Relay (1.0)
logp	1.008		Crippen Method
mcvol	147.880	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1173.00		NIST Webbook
tb	476.10	K	Cheméo Relay (1.0)
tc	619.41	K	Cheméo Relay (1.0)
tf	295.88	K	Cheméo Relay (1.0)
vc	0.541	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.67	J/mol×K	557.35	Joback Method
cpg	384.63	J/mol×K	586.10	Joback Method
cpg	395.03	J/mol×K	614.84	Joback Method
cpg	404.88	J/mol×K	643.59	Joback Method
cpg	414.21	J/mol×K	672.33	Joback Method
cpg	423.03	J/mol×K	701.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C764169&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):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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