Propanoic acid, 3-amino-2-methyl, butyl ester, TFA

Inchi: InChI=1S/C10H16F3NO3/c1-3-4-5-17-8(15)7(2)6-14-9(16)10(11,12)13/h7H,3-6H2,1-2H3

InchiKey: JKIYRYDLTOXQAQ-UHFFFAOYSA-N

Formula: C10H16F3NO3

SMILES: CCCCOC(=O)C(C)CNC(=O)C(F)(F)F

Mol. weight [g/mol]: 255.23

CAS: 54986-69-5

Physical Properties

Property code	Value	Unit	Source
gf	-824.16	kJ/mol	Joback Method
hf	-1156.00	kJ/mol	Joback Method
hfus	29.44	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.644		Crippen Method
mcvol	176.060	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1282.00		NIST Webbook
tb	602.67	K	Joback Method
tc	775.83	K	Joback Method
tf	366.40	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.69	J/mol×K	602.67	Joback Method
cpg	482.24	J/mol×K	631.53	Joback Method
cpg	494.15	J/mol×K	660.39	Joback Method
cpg	505.42	J/mol×K	689.25	Joback Method
cpg	516.08	J/mol×K	718.11	Joback Method
cpg	526.14	J/mol×K	746.97	Joback Method
cpg	535.63	J/mol×K	775.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54986695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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