3-Amino-1-propanol, N,O-di(trifluoroacetyl)-

Inchi: InChI=1S/C7H7F6NO3/c8-6(9,10)4(15)14-2-1-3-17-5(16)7(11,12)13/h1-3H2,(H,14,15)
InchiKey: KMHISLALRBUFCH-UHFFFAOYSA-N
Formula: C7H7F6NO3
SMILES: O=C(NCCCOC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 267.13

Physical Properties

Property code	Value	Unit	Source
gf	-1428.57	kJ/mol	Joback Method
hf	-1685.88	kJ/mol	Joback Method
hfus	27.02	kJ/mol	Joback Method
hvap	46.02	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.161		Crippen Method
mcvol	139.100	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1059.00		NIST Webbook
rinpol	1059.00		NIST Webbook
tb	529.05	K	Joback Method
tc	689.90	K	Joback Method
tf	351.78	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.78	J/mol×K	529.05	Joback Method
cpg	366.30	J/mol×K	555.86	Joback Method
cpg	375.25	J/mol×K	582.67	Joback Method
cpg	383.68	J/mol×K	609.47	Joback Method
cpg	391.58	J/mol×K	636.28	Joback Method
cpg	399.00	J/mol×K	663.09	Joback Method
cpg	405.95	J/mol×K	689.90	Joback Method

Sources

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=U374890&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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