6-Amino-1-hexanol, N,O-bis(trifluoroacetyl)-

Inchi: InChI=1S/C10H13F6NO3/c11-9(12,13)7(18)17-5-3-1-2-4-6-20-8(19)10(14,15)16/h1-6H2,
InchiKey: RJZPKKUQEKOKLE-UHFFFAOYSA-N
Formula: C10H13F6NO3
SMILES: O=C(NCCCCCCOC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 309.21

Physical Properties

Property code	Value	Unit	Source
gf	-1403.31	kJ/mol	Joback Method
hf	-1747.80	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	52.70	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.331		Crippen Method
mcvol	181.370	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1349.00		NIST Webbook
rinpol	1349.00		NIST Webbook
tb	597.69	K	Joback Method
tc	757.54	K	Joback Method
tf	385.59	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.97	J/mol×K	597.69	Joback Method
cpg	508.40	J/mol×K	624.33	Joback Method
cpg	519.20	J/mol×K	650.97	Joback Method
cpg	529.39	J/mol×K	677.62	Joback Method
cpg	539.00	J/mol×K	704.26	Joback Method
cpg	548.05	J/mol×K	730.90	Joback Method
cpg	556.57	J/mol×K	757.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375565&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

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