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

Inchi: InChI=1S/C9H7F10NO3/c10-6(11,8(14,15)16)4(21)20-2-1-3-23-5(22)7(12,13)9(17,18)19

InchiKey: MZRZYRSHHYXUFP-UHFFFAOYSA-N

Formula: C9H7F10NO3

SMILES: O=C(NCCCOC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 367.14

Physical Properties

Property code	Value	Unit	Source
gf	-2185.29	kJ/mol	Joback Method
hf	-2529.10	kJ/mol	Joback Method
hfus	29.69	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.431		Crippen Method
mcvol	174.360	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	1066.00		NIST Webbook
tb	565.43	K	Joback Method
tc	716.32	K	Joback Method
tf	381.52	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.28	J/mol×K	565.43	Joback Method
cpg	498.54	J/mol×K	590.58	Joback Method
cpg	508.10	J/mol×K	615.73	Joback Method
cpg	517.01	J/mol×K	640.88	Joback Method
cpg	525.29	J/mol×K	666.03	Joback Method
cpg	532.99	J/mol×K	691.17	Joback Method
cpg	540.14	J/mol×K	716.32	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=U374891&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