5-amino-1-pentanol, N,O-bis(pentafluoropropionyl)-

Inchi: InChI=1S/C11H11F10NO3/c12-8(13,10(16,17)18)6(23)22-4-2-1-3-5-25-7(24)9(14,15)11(

InchiKey: XDWOIGHLCVMKKS-UHFFFAOYSA-N

Formula: C11H11F10NO3

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

Mol. weight [g/mol]: 395.19

Physical Properties

Property code	Value	Unit	Source
gf	-2168.45	kJ/mol	Joback Method
hf	-2570.38	kJ/mol	Joback Method
hfus	34.87	kJ/mol	Joback Method
hvap	49.06	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.211		Crippen Method
mcvol	202.540	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	1279.00		NIST Webbook
tb	611.19	K	Joback Method
tc	763.56	K	Joback Method
tf	404.06	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.52	J/mol×K	611.19	Joback Method
cpg	596.72	J/mol×K	636.59	Joback Method
cpg	607.18	J/mol×K	661.98	Joback Method
cpg	616.97	J/mol×K	687.38	Joback Method
cpg	626.11	J/mol×K	712.77	Joback Method
cpg	634.65	J/mol×K	738.17	Joback Method
cpg	642.62	J/mol×K	763.56	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=U374917&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