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

Inchi: InChI=1S/C11H7F14NO3/c12-6(13,8(16,17)10(20,21)22)4(27)26-2-1-3-29-5(28)7(14,15)9(18,19)11(23,24)25/h1-3H2,(H,26,27)

InchiKey: DWCOAJWZQZMFTA-UHFFFAOYSA-N

Formula: C11H7F14NO3

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

Mol. weight [g/mol]: 467.16

Physical Properties

Property code	Value	Unit	Source
gf	-2942.01	kJ/mol	Joback Method
hf	-3372.32	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	43.20	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.702		Crippen Method
mcvol	209.620	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	1137.00		NIST Webbook
rinpol	1137.00		NIST Webbook
tb	601.81	K	Joback Method
tc	747.44	K	Joback Method
tf	411.26	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.46	J/mol×K	601.81	Joback Method
cpg	635.06	J/mol×K	626.08	Joback Method
cpg	644.86	J/mol×K	650.35	Joback Method
cpg	653.93	J/mol×K	674.62	Joback Method
cpg	662.30	J/mol×K	698.90	Joback Method
cpg	670.03	J/mol×K	723.17	Joback Method
cpg	677.17	J/mol×K	747.44	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=U374892&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