«beta»-Alanine, n-heptafluorobutyryl-, pentyl ester

Inchi: InChI=1S/C12H16F7NO3/c1-2-3-4-7-23-8(21)5-6-20-9(22)10(13,14)11(15,16)12(17,18)1

InchiKey: PVONQJZVLUWSGW-UHFFFAOYSA-N

Formula: C12H16F7NO3

SMILES: CCCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 355.25

Physical Properties

Property code	Value	Unit	Source
gf	-1578.44	kJ/mol	Joback Method
hf	-1993.94	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	55.04	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.059		Crippen Method
mcvol	211.320	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
tb	639.49	K	Joback Method
tc	800.76	K	Joback Method
tf	411.14	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.96	J/mol×K	639.49	Joback Method
cpg	621.37	J/mol×K	666.37	Joback Method
cpg	633.03	J/mol×K	693.25	Joback Method
cpg	643.99	J/mol×K	720.12	Joback Method
cpg	654.29	J/mol×K	747.00	Joback Method
cpg	663.96	J/mol×K	773.88	Joback Method
cpg	673.04	J/mol×K	800.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320980&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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