«beta»-Alanine, n-pentafluoropropionyl-, hexyl ester

Inchi: InChI=1S/C12H18F5NO3/c1-2-3-4-5-8-21-9(19)6-7-18-10(20)11(13,14)12(15,16)17/h2-8

InchiKey: CPXNIJLLOKWCQL-UHFFFAOYSA-N

Formula: C12H18F5NO3

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

Mol. weight [g/mol]: 319.27

Physical Properties

Property code	Value	Unit	Source
gf	-1191.66	kJ/mol	Joback Method
hf	-1592.97	kJ/mol	Joback Method
hfus	36.89	kJ/mol	Joback Method
hvap	57.97	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.814		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1484.00		NIST Webbook
tb	644.18	K	Joback Method
tc	809.46	K	Joback Method
tf	407.54	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.92	J/mol×K	644.18	Joback Method
cpg	602.82	J/mol×K	671.73	Joback Method
cpg	615.00	J/mol×K	699.27	Joback Method
cpg	626.50	J/mol×K	726.82	Joback Method
cpg	637.35	J/mol×K	754.37	Joback Method
cpg	647.57	J/mol×K	781.92	Joback Method
cpg	657.21	J/mol×K	809.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320952&Units=SI

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