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

Inchi: InChI=1S/C12H18F5NO3/c1-8(2)4-3-7-21-9(19)5-6-18-10(20)11(13,14)12(15,16)17/h8H,

InchiKey: QGWMGCPJHYKYJS-UHFFFAOYSA-N

Formula: C12H18F5NO3

SMILES: CC(C)CCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 319.27

Physical Properties

Property code	Value	Unit	Source
gf	-1194.10	kJ/mol	Joback Method
hf	-1598.25	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	57.58	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.670		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1436.00		NIST Webbook
tb	643.74	K	Joback Method
tc	811.12	K	Joback Method
tf	392.54	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.38	J/mol×K	643.74	Joback Method
cpg	603.47	J/mol×K	671.64	Joback Method
cpg	615.83	J/mol×K	699.53	Joback Method
cpg	627.48	J/mol×K	727.43	Joback Method
cpg	638.46	J/mol×K	755.33	Joback Method
cpg	648.80	J/mol×K	783.22	Joback Method
cpg	658.52	J/mol×K	811.12	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=U320951&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