.beta.-Alanine, N-pentafluoropropionyl-, heptyl ester

Inchi: InChI=1S/C13H20F5NO3/c1-2-3-4-5-6-9-22-10(20)7-8-19-11(21)12(14,15)13(16,17)18/h

InchiKey: WKDQUYFPTJNDAN-UHFFFAOYSA-N

Formula: C13H20F5NO3

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

Mol. weight [g/mol]: 333.30

Physical Properties

Property code	Value	Unit	Source
hf	-1790.06	kJ/mol	Cheméo Relay (1.0)
hfus	39.48	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.24		Cheméo Relay (1.0)
logp	3.204		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	1572.00		NIST Webbook
tb	524.95	K	Cheméo Relay (1.0)
tc	665.13	K	Cheméo Relay (1.0)
tf	292.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.47	J/mol×K	667.06	Joback Method
cpg	655.84	J/mol×K	694.69	Joback Method
cpg	668.48	J/mol×K	722.33	Joback Method
cpg	680.41	J/mol×K	749.96	Joback Method
cpg	691.67	J/mol×K	777.59	Joback Method
cpg	702.29	J/mol×K	805.22	Joback Method
cpg	712.30	J/mol×K	832.86	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320953&Units=SI

Legend

cpg:	Ideal gas heat capacity
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