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

Inchi: InChI=1S/C17H28F5NO3/c1-2-3-4-5-6-7-8-9-10-13-26-14(24)11-12-23-15(25)16(18,19)1

InchiKey: ZSEBBVAQLWHJMQ-UHFFFAOYSA-N

Formula: C17H28F5NO3

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

Mol. weight [g/mol]: 389.40

Physical Properties

Property code	Value	Unit	Source
gf	-1149.56	kJ/mol	Joback Method
hf	-1696.17	kJ/mol	Joback Method
hfus	49.84	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.764		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	1952.00		NIST Webbook
tb	758.58	K	Joback Method
tc	931.61	K	Joback Method
tf	463.89	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.18	J/mol×K	758.58	Joback Method
cpg	879.42	J/mol×K	787.42	Joback Method
cpg	893.81	J/mol×K	816.26	Joback Method
cpg	907.37	J/mol×K	845.10	Joback Method
cpg	920.17	J/mol×K	873.93	Joback Method
cpg	932.23	J/mol×K	902.77	Joback Method
cpg	943.61	J/mol×K	931.61	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=U320956&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