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

Inchi: InChI=1S/C9H12F5NO3/c1-2-5-18-6(16)3-4-15-7(17)8(10,11)9(12,13)14/h2-5H2,1H3,(H,
InchiKey: ZAVDUJUNBMRPLS-UHFFFAOYSA-N
Formula: C9H12F5NO3
SMILES: CCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 277.19

Physical Properties

Property code	Value	Unit	Source
gf	-1216.92	kJ/mol	Joback Method
hf	-1531.05	kJ/mol	Joback Method
hfus	29.12	kJ/mol	Joback Method
hvap	51.29	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.643		Crippen Method
mcvol	165.510	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1202.00		NIST Webbook
tb	575.54	K	Joback Method
tc	741.52	K	Joback Method
tf	373.73	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.45	J/mol×K	575.54	Joback Method
cpg	451.72	J/mol×K	603.20	Joback Method
cpg	462.35	J/mol×K	630.87	Joback Method
cpg	472.35	J/mol×K	658.53	Joback Method
cpg	481.77	J/mol×K	686.19	Joback Method
cpg	490.62	J/mol×K	713.86	Joback Method
cpg	498.94	J/mol×K	741.52	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=U320948&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