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

Inchi: InChI=1S/C23H40F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-32-20(30)17-18-2

InchiKey: SVPAUDRNJZGLSS-UHFFFAOYSA-N

Formula: C23H40F5NO3

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

Mol. weight [g/mol]: 473.56

Physical Properties

Property code	Value	Unit	Source
gf	-1099.04	kJ/mol	Joback Method
hf	-1820.01	kJ/mol	Joback Method
hfus	65.38	kJ/mol	Joback Method
hvap	82.45	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	7.105		Crippen Method
mcvol	362.770	ml/mol	McGowan Method
pc	820.54	kPa	Joback Method
rinpol	2536.00		NIST Webbook
tb	895.86	K	Joback Method
tc	1102.14	K	Joback Method
tf	531.51	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.97	J/mol×K	895.86	Joback Method
cpg	1242.89	J/mol×K	930.24	Joback Method
cpg	1260.59	J/mol×K	964.62	Joback Method
cpg	1277.17	J/mol×K	999.00	Joback Method
cpg	1292.71	J/mol×K	1033.38	Joback Method
cpg	1307.31	J/mol×K	1067.76	Joback Method
cpg	1321.05	J/mol×K	1102.14	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=U320961&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