«beta»-Alanine, n-heptafluorobutyryl-, pentadecyl ester

Inchi: InChI=1S/C22H36F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-33-18(31)15-16-30-19(3

InchiKey: YDKZHIHXGNPMQC-UHFFFAOYSA-N

Formula: C22H36F7NO3

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

Mol. weight [g/mol]: 495.51

Physical Properties

Property code	Value	Unit	Source
gf	-1494.24	kJ/mol	Joback Method
hf	-2200.34	kJ/mol	Joback Method
hfus	61.54	kJ/mol	Joback Method
hvap	77.30	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	6.960		Crippen Method
mcvol	352.220	ml/mol	McGowan Method
pc	832.42	kPa	Joback Method
rinpol	2365.00		NIST Webbook
tb	868.29	K	Joback Method
tc	1066.85	K	Joback Method
tf	523.84	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.07	J/mol×K	868.29	Joback Method
cpg	1194.86	J/mol×K	901.38	Joback Method
cpg	1211.53	J/mol×K	934.48	Joback Method
cpg	1227.19	J/mol×K	967.57	Joback Method
cpg	1241.94	J/mol×K	1000.67	Joback Method
cpg	1255.88	J/mol×K	1033.76	Joback Method
cpg	1269.09	J/mol×K	1066.85	Joback Method

Sources

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=U320986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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