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

Inchi: InChI=1S/C22H38F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-31-19(29)16-17-28-2

InchiKey: ZKBLPPOCZRMOPK-UHFFFAOYSA-N

Formula: C22H38F5NO3

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

Mol. weight [g/mol]: 459.53

Physical Properties

Property code	Value	Unit	Source
gf	-1107.46	kJ/mol	Joback Method
hf	-1799.37	kJ/mol	Joback Method
hfus	62.79	kJ/mol	Joback Method
hvap	80.23	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	6.715		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
pc	867.60	kPa	Joback Method
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
tb	872.98	K	Joback Method
tc	1071.32	K	Joback Method
tf	520.24	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.17	J/mol×K	872.98	Joback Method
cpg	1180.34	J/mol×K	906.04	Joback Method
cpg	1197.38	J/mol×K	939.09	Joback Method
cpg	1213.35	J/mol×K	972.15	Joback Method
cpg	1228.35	J/mol×K	1005.21	Joback Method
cpg	1242.44	J/mol×K	1038.27	Joback Method
cpg	1255.71	J/mol×K	1071.32	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=U320960&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