.beta.-Alanine, N-heptafluorobutyryl-, hexyl ester

Inchi: InChI=1S/C13H18F7NO3/c1-2-3-4-5-8-24-9(22)6-7-21-10(23)11(14,15)12(16,17)13(18,1

InchiKey: HOGAAYZDAGRTRS-UHFFFAOYSA-N

Formula: C13H18F7NO3

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

Mol. weight [g/mol]: 369.28

Physical Properties

Property code	Value	Unit	Source
hf	-2180.59	kJ/mol	Cheméo Relay (1.0)
hfus	38.23	kJ/mol	Joback Method
hvap	75.59	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.68		Cheméo Relay (1.0)
logp	3.449		Crippen Method
mcvol	225.410	ml/mol	McGowan Method
rinpol	1511.00		NIST Webbook
tb	521.48	K	Cheméo Relay (1.0)
tc	655.78	K	Cheméo Relay (1.0)
tf	276.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.18	J/mol×K	662.37	Joback Method
cpg	674.03	J/mol×K	689.39	Joback Method
cpg	686.12	J/mol×K	716.42	Joback Method
cpg	697.50	J/mol×K	743.44	Joback Method
cpg	708.20	J/mol×K	770.46	Joback Method
cpg	718.26	J/mol×K	797.49	Joback Method
cpg	727.72	J/mol×K	824.51	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320981&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point