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

Inchi: InChI=1S/C23H38F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-34-19(32)16-17-31-2

InchiKey: KYDONHMBRSQUMJ-UHFFFAOYSA-N

Formula: C23H38F7NO3

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

Mol. weight [g/mol]: 509.55

Physical Properties

Property code	Value	Unit	Source
hf	-2374.45	kJ/mol	Cheméo Relay (1.0)
hfus	64.13	kJ/mol	Joback Method
hvap	115.50	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.78		Cheméo Relay (1.0)
logp	7.350		Crippen Method
mcvol	366.310	ml/mol	McGowan Method
rinpol	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook
tb	626.48	K	Cheméo Relay (1.0)
tc	753.66	K	Cheméo Relay (1.0)
tf	319.96	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.46	J/mol×K	891.17	Joback Method
cpg	1257.05	J/mol×K	925.68	Joback Method
cpg	1274.47	J/mol×K	960.18	Joback Method
cpg	1290.82	J/mol×K	994.69	Joback Method
cpg	1306.22	J/mol×K	1029.19	Joback Method
cpg	1320.77	J/mol×K	1063.70	Joback Method
cpg	1334.60	J/mol×K	1098.21	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=U320987&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