.BETA.-alanine, n-heptafluorobutyryl-, tetradecyl ester

Inchi: InChI=1S/C21H34F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-32-17(30)14-15-29-18(31)1

InchiKey: HZXRIAXXRDQPLP-UHFFFAOYSA-N

Formula: C21H34F7NO3

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

Mol. weight [g/mol]: 481.49

Physical Properties

Property code	Value	Unit	Source
hf	-2335.51	kJ/mol	Cheméo Relay (1.0)
hfus	58.95	kJ/mol	Joback Method
hvap	107.81	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.25		Cheméo Relay (1.0)
logp	6.570		Crippen Method
mcvol	338.130	ml/mol	McGowan Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	608.95	K	Cheméo Relay (1.0)
tc	735.81	K	Cheméo Relay (1.0)
tf	312.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.37	J/mol×K	845.41	Joback Method
cpg	1133.42	J/mol×K	877.27	Joback Method
cpg	1149.42	J/mol×K	909.14	Joback Method
cpg	1164.46	J/mol×K	941.00	Joback Method
cpg	1178.63	J/mol×K	972.86	Joback Method
cpg	1192.00	J/mol×K	1004.73	Joback Method
cpg	1204.67	J/mol×K	1036.59	Joback Method

Sources

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=U320985&Units=SI
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

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