L-phenylalanine, n-heptafluorobutyryl-, ethyl ester

Inchi: InChI=1S/C15H14F7NO3/c1-2-26-11(24)10(8-9-6-4-3-5-7-9)23-12(25)13(16,17)14(18,19

InchiKey: CCMIJEFRAULLGD-UHFFFAOYSA-N

Formula: C15H14F7NO3

SMILES: CCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 389.27

Physical Properties

Property code	Value	Unit	Source
hfus	33.93	kJ/mol	Joback Method
log10ws	-4.66		Cheméo Relay (1.0)
logp	3.110		Crippen Method
mcvol	229.830	ml/mol	McGowan Method
rinpol	1568.00		NIST Webbook
tb	552.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.37	J/mol×K	734.37	Joback Method
cpg	696.40	J/mol×K	765.44	Joback Method
cpg	707.50	J/mol×K	796.51	Joback Method
cpg	717.76	J/mol×K	827.58	Joback Method
cpg	727.25	J/mol×K	858.65	Joback Method
cpg	736.03	J/mol×K	889.72	Joback Method
cpg	744.18	J/mol×K	920.79	Joback Method

Sources

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=U321107&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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