L-Phenylalanine, N-heptafluorobutyryl-, nonyl ester

Inchi: InChI=1S/C22H28F7NO3/c1-2-3-4-5-6-7-11-14-33-18(31)17(15-16-12-9-8-10-13-16)30-1

InchiKey: LCYCKEDIQPLGIT-UHFFFAOYSA-N

Formula: C22H28F7NO3

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

Mol. weight [g/mol]: 487.46

Physical Properties

Property code	Value	Unit	Source
hfus	52.06	kJ/mol	Joback Method
log10ws	-6.87		Cheméo Relay (1.0)
logp	5.841		Crippen Method
mcvol	328.460	ml/mol	McGowan Method
pc	1022.69	kPa	Joback Method
rinpol	2191.00		NIST Webbook
tb	630.02	K	Cheméo Relay (1.0)
tf	319.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1080.75	J/mol×K	894.53	Joback Method
cpg	1095.36	J/mol×K	927.98	Joback Method
cpg	1109.00	J/mol×K	961.42	Joback Method
cpg	1121.78	J/mol×K	994.87	Joback Method
cpg	1133.79	J/mol×K	1028.32	Joback Method
cpg	1145.15	J/mol×K	1061.77	Joback Method
cpg	1155.95	J/mol×K	1095.21	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=U321113&Units=SI

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point