L-Phenylalanine, N-pentafluoropropionyl-, butyl ester

Inchi: InChI=1S/C16H18F5NO3/c1-2-3-9-25-13(23)12(10-11-7-5-4-6-8-11)22-14(24)15(17,18)1

InchiKey: AYCLHSDTIGUZDL-UHFFFAOYSA-N

Formula: C16H18F5NO3

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

Mol. weight [g/mol]: 367.31

Physical Properties

Property code	Value	Unit	Source
af	0.7092		Cheméo Relay (1.0)
hfus	37.77	kJ/mol	Joback Method
log10ws	-4.59		Cheméo Relay (1.0)
logp	3.255		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook
tb	567.21	K	Cheméo Relay (1.0)
tc	733.35	K	Cheméo Relay (1.0)
tf	312.77	K	Cheméo Relay (1.0)
vc	0.854	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.72	J/mol×K	761.94	Joback Method
cpg	733.76	J/mol×K	793.70	Joback Method
cpg	745.86	J/mol×K	825.46	Joback Method
cpg	757.10	J/mol×K	857.22	Joback Method
cpg	767.53	J/mol×K	888.98	Joback Method
cpg	777.22	J/mol×K	920.74	Joback Method
cpg	786.21	J/mol×K	952.51	Joback Method

Sources

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=U321020&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume