l-Phenylalanine, n-heptafluorobutyryl-, tetradecyl ester

Inchi: InChI=1S/C27H38F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-16-19-38-23(36)22(20-21-17-14-1

InchiKey: QWZVQXJJVOMLTI-UHFFFAOYSA-N

Formula: C27H38F7NO3

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

Mol. weight [g/mol]: 557.58

Physical Properties

Property code	Value	Unit	Source
gf	-1342.17	kJ/mol	Joback Method
hf	-2072.29	kJ/mol	Joback Method
hfus	65.01	kJ/mol	Joback Method
hvap	90.31	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	7.791		Crippen Method
mcvol	398.910	ml/mol	McGowan Method
pc	768.61	kPa	Joback Method
rinpol	2677.00		NIST Webbook
tb	1008.93	K	Joback Method
tc	1247.04	K	Joback Method
tf	591.61	K	Joback Method
vc	1.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1385.84	J/mol×K	1008.93	Joback Method
cpg	1403.82	J/mol×K	1048.61	Joback Method
cpg	1420.70	J/mol×K	1088.30	Joback Method
cpg	1436.67	J/mol×K	1127.98	Joback Method
cpg	1451.93	J/mol×K	1167.67	Joback Method
cpg	1466.69	J/mol×K	1207.35	Joback Method
cpg	1481.13	J/mol×K	1247.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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