l-Phenylalanine, n-heptafluorobutyryl-, heptadecyl ester

Inchi: InChI=1S/C30H44F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-41-26(39)25(23-2

InchiKey: PPJKZUYNOPPALL-UHFFFAOYSA-N

Formula: C30H44F7NO3

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

Mol. weight [g/mol]: 599.66

Physical Properties

Property code	Value	Unit	Source
gf	-1316.91	kJ/mol	Joback Method
hf	-2134.21	kJ/mol	Joback Method
hfus	72.78	kJ/mol	Joback Method
hvap	96.99	kJ/mol	Joback Method
log10ws	-10.71		Crippen Method
logp	8.961		Crippen Method
mcvol	441.180	ml/mol	McGowan Method
pc	659.15	kPa	Joback Method
rinpol	3063.00		NIST Webbook
tb	1077.57	K	Joback Method
tc	1353.96	K	Joback Method
tf	625.42	K	Joback Method
vc	1.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1575.78	J/mol×K	1077.57	Joback Method
cpg	1597.06	J/mol×K	1123.63	Joback Method
cpg	1617.18	J/mol×K	1169.70	Joback Method
cpg	1636.46	J/mol×K	1215.76	Joback Method
cpg	1655.25	J/mol×K	1261.83	Joback Method
cpg	1673.86	J/mol×K	1307.89	Joback Method
cpg	1692.63	J/mol×K	1353.96	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321120&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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