l-Phenylalanine, n-heptafluorobutyryl-, decyl ester

Inchi: InChI=1S/C23H30F7NO3/c1-2-3-4-5-6-7-8-12-15-34-19(32)18(16-17-13-10-9-11-14-17)3

InchiKey: SQFRBKMGMQFRTF-UHFFFAOYSA-N

Formula: C23H30F7NO3

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

Mol. weight [g/mol]: 501.48

Physical Properties

Property code	Value	Unit	Source
gf	-1375.85	kJ/mol	Joback Method
hf	-1989.73	kJ/mol	Joback Method
hfus	54.65	kJ/mol	Joback Method
hvap	81.41	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	6.231		Crippen Method
mcvol	342.550	ml/mol	McGowan Method
pc	962.67	kPa	Joback Method
rinpol	2288.00		NIST Webbook
rinpol	2288.00		NIST Webbook
tb	917.41	K	Joback Method
tc	1123.38	K	Joback Method
tf	546.53	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.50	J/mol×K	917.41	Joback Method
cpg	1155.64	J/mol×K	951.74	Joback Method
cpg	1169.78	J/mol×K	986.07	Joback Method
cpg	1183.04	J/mol×K	1020.39	Joback Method
cpg	1195.54	J/mol×K	1054.72	Joback Method
cpg	1207.40	J/mol×K	1089.05	Joback Method
cpg	1218.73	J/mol×K	1123.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321114&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