l-Phenylalanine, n-heptafluorobutyryl-, dodecyl ester

Inchi: InChI=1S/C25H34F7NO3/c1-2-3-4-5-6-7-8-9-10-14-17-36-21(34)20(18-19-15-12-11-13-1

InchiKey: RSPXMXUFHOUQCC-UHFFFAOYSA-N

Formula: C25H34F7NO3

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

Mol. weight [g/mol]: 529.53

Physical Properties

Property code	Value	Unit	Source
gf	-1359.01	kJ/mol	Joback Method
hf	-2031.01	kJ/mol	Joback Method
hfus	59.83	kJ/mol	Joback Method
hvap	85.86	kJ/mol	Joback Method
log10ws	-8.62		Crippen Method
logp	7.011		Crippen Method
mcvol	370.730	ml/mol	McGowan Method
pc	857.47	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	963.17	K	Joback Method
tc	1182.84	K	Joback Method
tf	569.07	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1261.97	J/mol×K	963.17	Joback Method
cpg	1278.35	J/mol×K	999.78	Joback Method
cpg	1293.68	J/mol×K	1036.39	Joback Method
cpg	1308.12	J/mol×K	1073.00	Joback Method
cpg	1321.81	J/mol×K	1109.62	Joback Method
cpg	1334.90	J/mol×K	1146.23	Joback Method
cpg	1347.54	J/mol×K	1182.84	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321116&Units=SI

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