l-Phenylalanine, n-heptafluorobutyryl-, pentyl ester

Inchi: InChI=1S/C18H20F7NO3/c1-2-3-7-10-29-14(27)13(11-12-8-5-4-6-9-12)26-15(28)16(19,2

InchiKey: IWPULFBBUCUDMG-UHFFFAOYSA-N

Formula: C18H20F7NO3

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

Mol. weight [g/mol]: 431.35

Physical Properties

Property code	Value	Unit	Source
gf	-1417.95	kJ/mol	Joback Method
hf	-1886.53	kJ/mol	Joback Method
hfus	41.70	kJ/mol	Joback Method
hvap	70.28	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.280		Crippen Method
mcvol	272.100	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	803.01	K	Joback Method
tc	991.29	K	Joback Method
tf	490.18	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.10	J/mol×K	803.01	Joback Method
cpg	862.10	J/mol×K	834.39	Joback Method
cpg	874.18	J/mol×K	865.77	Joback Method
cpg	885.42	J/mol×K	897.15	Joback Method
cpg	895.89	J/mol×K	928.53	Joback Method
cpg	905.68	J/mol×K	959.91	Joback Method
cpg	914.86	J/mol×K	991.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321110&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