l-Phenylalanine, n-pentafluoropropionyl-, octyl ester

Inchi: InChI=1S/C20H26F5NO3/c1-2-3-4-5-6-10-13-29-17(27)16(14-15-11-8-7-9-12-15)26-18(2

InchiKey: PHECSIOHURIUHP-UHFFFAOYSA-N

Formula: C20H26F5NO3

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

Mol. weight [g/mol]: 423.42

Physical Properties

Property code	Value	Unit	Source
gf	-1014.33	kJ/mol	Joback Method
hf	-1526.84	kJ/mol	Joback Method
hfus	48.13	kJ/mol	Joback Method
hvap	77.66	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.815		Crippen Method
mcvol	296.740	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	853.46	K	Joback Method
tc	1048.66	K	Joback Method
tf	509.12	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.59	J/mol×K	853.46	Joback Method
cpg	961.92	J/mol×K	885.99	Joback Method
cpg	975.27	J/mol×K	918.53	Joback Method
cpg	987.71	J/mol×K	951.06	Joback Method
cpg	999.32	J/mol×K	983.59	Joback Method
cpg	1010.17	J/mol×K	1016.13	Joback Method
cpg	1020.33	J/mol×K	1048.66	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=U321023&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