l-Phenylalanine, n-pentafluoropropionyl-, heptadecyl ester

Inchi: InChI=1S/C29H44F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-38-26(36)25(23-2

InchiKey: DYEVCFBWRFGXBK-UHFFFAOYSA-N

Formula: C29H44F5NO3

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

Mol. weight [g/mol]: 549.66

Physical Properties

Property code	Value	Unit	Source
gf	-938.55	kJ/mol	Joback Method
hf	-1712.60	kJ/mol	Joback Method
hfus	71.44	kJ/mol	Joback Method
hvap	97.70	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	8.326		Crippen Method
mcvol	423.550	ml/mol	McGowan Method
pc	719.53	kPa	Joback Method
rinpol	3055.00		NIST Webbook
rinpol	3055.00		NIST Webbook
tb	1059.38	K	Joback Method
tc	1318.63	K	Joback Method
tf	610.55	K	Joback Method
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1498.99	J/mol×K	1059.38	Joback Method
cpg	1518.76	J/mol×K	1102.59	Joback Method
cpg	1537.16	J/mol×K	1145.80	Joback Method
cpg	1554.42	J/mol×K	1189.00	Joback Method
cpg	1570.77	J/mol×K	1232.21	Joback Method
cpg	1586.44	J/mol×K	1275.42	Joback Method
cpg	1601.66	J/mol×K	1318.63	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=U321031&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

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