l-Phenylalanine, n-heptafluorobutyryl-, pentadecyl ester

Inchi: InChI=1S/C28H40F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-39-24(37)23(21-22-18-1

InchiKey: QWZNASQTTVGIIH-UHFFFAOYSA-N

Formula: C28H40F7NO3

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

Mol. weight [g/mol]: 571.61

Physical Properties

Property code	Value	Unit	Source
gf	-1333.75	kJ/mol	Joback Method
hf	-2092.93	kJ/mol	Joback Method
hfus	67.60	kJ/mol	Joback Method
hvap	92.54	kJ/mol	Joback Method
log10ws	-9.88		Crippen Method
logp	8.181		Crippen Method
mcvol	413.000	ml/mol	McGowan Method
pc	729.28	kPa	Joback Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
tb	1031.81	K	Joback Method
tc	1281.15	K	Joback Method
tf	602.88	K	Joback Method
vc	1.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1448.62	J/mol×K	1031.81	Joback Method
cpg	1467.56	J/mol×K	1073.37	Joback Method
cpg	1485.38	J/mol×K	1114.92	Joback Method
cpg	1502.29	J/mol×K	1156.48	Joback Method
cpg	1518.55	J/mol×K	1198.04	Joback Method
cpg	1534.37	J/mol×K	1239.59	Joback Method
cpg	1549.99	J/mol×K	1281.15	Joback Method

Sources

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=U321118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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