l-Phenylalanine, n-heptafluorobutyryl-, propyl ester

Inchi: InChI=1S/C16H16F7NO3/c1-2-8-27-12(25)11(9-10-6-4-3-5-7-10)24-13(26)14(17,18)15(1

InchiKey: BENJCXJHHRAYLJ-UHFFFAOYSA-N

Formula: C16H16F7NO3

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

Mol. weight [g/mol]: 403.29

Physical Properties

Property code	Value	Unit	Source
gf	-1434.79	kJ/mol	Joback Method
hf	-1845.25	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	65.83	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.500		Crippen Method
mcvol	243.920	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	757.25	K	Joback Method
tc	943.70	K	Joback Method
tf	467.64	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.32	J/mol×K	757.25	Joback Method
cpg	750.67	J/mol×K	788.32	Joback Method
cpg	762.10	J/mol×K	819.40	Joback Method
cpg	772.68	J/mol×K	850.47	Joback Method
cpg	782.50	J/mol×K	881.55	Joback Method
cpg	791.62	J/mol×K	912.62	Joback Method
cpg	800.11	J/mol×K	943.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321108&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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