

L-Phenylalanine, N-heptafluorobutyryl-, hexadecyl ester

Inchi: InChI=1S/C29H42F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-40-25(38)24(22-23-1
InchiKey: GPYLMDHCDSEFFLE-UHFFFAOYSA-N
Formula: C29H42F7NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 585.65

Physical Properties

Property code	Value	Unit	Source
hfus	70.19	kJ/mol	Joback Method
log10ws	-8.79		Cheméo Relay (1.0)
logp	8.571		Crippen Method
mcvol	427.090	ml/mol	McGowan Method
pc	692.89	kPa	Joback Method
rinpol	2915.00		NIST Webbook
tb	686.76	K	Cheméo Relay (1.0)
tf	331.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.94	J/mol×K	1054.69	Joback Method
cpg	1531.98	J/mol×K	1098.37	Joback Method
cpg	1550.86	J/mol×K	1142.04	Joback Method
cpg	1568.87	J/mol×K	1185.72	Joback Method
cpg	1586.29	J/mol×K	1229.40	Joback Method
cpg	1603.37	J/mol×K	1273.07	Joback Method
cpg	1620.41	J/mol×K	1316.75	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321119&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point

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