

L-Valine, N-pentafluoropropionyl-, pentadecyl ester

Inchi:	InChI=1S/C23H40F5NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-32-20(30)19(18(2)3)2
InchiKey:	HTYUIPVJJQHEQW-UHFFFAOYSA-N
Formula:	C23H40F5NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]:	473.57

Physical Properties

Property code	Value	Unit	Source
hfus	58.34	kJ/mol	Joback Method
hvap	109.53	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.43		Cheméo Relay (1.0)
logp	6.959		Crippen Method
mcvol	362.770	ml/mol	McGowan Method
rinpol	2333.00		NIST Webbook
tb	594.63	K	Cheméo Relay (1.0)
tf	353.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.86	J/mol×K	894.98	Joback Method
cpg	1243.52	J/mol×K	928.96	Joback Method
cpg	1260.97	J/mol×K	962.94	Joback Method
cpg	1277.29	J/mol×K	996.92	Joback Method
cpg	1292.57	J/mol×K	1030.90	Joback Method
cpg	1306.90	J/mol×K	1064.88	Joback Method
cpg	1320.36	J/mol×K	1098.86	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320889&Units=SI
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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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