

L-Valine, N-pentafluorobenzoyl-, isobutyl ester

Inchi:	InChI=1S/C16H18F5NO3/c1-6(2)5-25-16(24)14(7(3)4)22-15(23)8-9(17)11(19)13(21)12(2
InchiKey:	UHCDBZBYCIDLSU-UHFFFAOYSA-N
Formula:	C16H18F5NO3
SMILES:	CC(C)COC(=O)C(NC(=O)c1c(F)c(F)c(F)c(F)c1F)C(C)C
Mol. weight [g/mol]:	367.31

Physical Properties

Property code	Value	Unit	Source
gf	-1106.72	kJ/mol	Joback Method
hf	-1494.69	kJ/mol	Joback Method
hfus	43.61	kJ/mol	Joback Method
hvap	73.88	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	3.336		Crippen Method
mvol	240.380	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	792.42	K	Joback Method
tc	980.85	K	Joback Method
tf	491.80	K	Joback Method
vc	0.961	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.83	J/molxK	792.42	Joback Method
cpg	725.53	J/molxK	823.82	Joback Method
cpg	737.38	J/molxK	855.23	Joback Method
cpg	748.41	J/molxK	886.63	Joback Method
cpg	758.62	J/molxK	918.04	Joback Method
cpg	768.02	J/molxK	949.44	Joback Method
cpg	776.60	J/molxK	980.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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