

I-Valine, n-heptafluorobutyryl-, isobutyl ester

Other names:	Val, isobutyl ester, HFB
	Val, iso-Bu, HFB
Inchi:	InChI=1S/C13H18F7NO3/c1-6(2)5-24-9(22)8(7(3)4)21-10(23)11(14,15)12(16,17)13(18,19)20
InchiKey:	DVJZJVCXAFDQLN-UHFFFAOYSA-N
Formula:	C13H18F7NO3
SMILES:	CC(C)COC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]:	369.28

Physical Properties

Property code	Value	Unit	Source
gf	-1577.34	kJ/mol	Joback Method
hf	-2030.42	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.159		Crippen Method
mcvol	225.410	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
tb	661.05	K	Joback Method
tc	828.60	K	Joback Method
tf	377.41	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.59	J/mol×K	661.05	Joback Method
cpg	675.98	J/mol×K	688.98	Joback Method
cpg	688.53	J/mol×K	716.90	Joback Method
cpg	700.30	J/mol×K	744.83	Joback Method
cpg	711.33	J/mol×K	772.75	Joback Method
cpg	721.66	J/mol×K	800.68	Joback Method
cpg	731.33	J/mol×K	828.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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