

# «beta»-Alanine, n-heptafluorobutyryl-, hexyl ester

Inchi:	InChI=1S/C13H18F7NO3/c1-2-3-4-5-8-24-9(22)6-7-21-10(23)11(14,15)12(16,17)13(18,1
InchiKey:	HOGAAYZDAGRTRS-UHFFFAOYSA-N
Formula:	C13H18F7NO3
SMILES:	CCCCCOC(=O)CCNC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	369.28

## Physical Properties

Property code	Value	Unit	Source
gf	-1570.02	kJ/mol	Joback Method
hf	-2014.58	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	57.26	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.449		Crippen Method
mvol	225.410	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rmpol	1511.00		NIST Webbook
tb	662.37	K	Joback Method
tc	824.51	K	Joback Method
tf	422.41	K	Joback Method
vc	0.921	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.18	J/mol×K	662.37	Joback Method
cpg	674.03	J/mol×K	689.39	Joback Method
cpg	686.12	J/mol×K	716.42	Joback Method
cpg	697.50	J/mol×K	743.44	Joback Method
cpg	708.20	J/mol×K	770.46	Joback Method
cpg	718.26	J/mol×K	797.49	Joback Method
cpg	727.72	J/mol×K	824.51	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U320981&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320981&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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