

# Sarcosine, n-pentafluorobenzoyl-, isohexyl ester

Inchi:	InChI=1S/C16H18F5NO3/c1-8(2)5-4-6-25-9(23)7-22(3)16(24)10-11(17)13(19)15(21)14(2)
InchiKey:	HSNLVAVTBKBYHA-UHFFFAOYSA-N
Formula:	C16H18F5NO3
SMILES:	CC(C)CCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	367.31

## Physical Properties

Property code	Value	Unit	Source
gf	-1080.45	kJ/mol	Joback Method
hf	-1470.07	kJ/mol	Joback Method
hfus	48.58	kJ/mol	Joback Method
hvap	70.27	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.433		Crippen Method
mvol	240.380	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	1930.00		NIST Webbook
tb	755.57	K	Joback Method
tc	935.85	K	Joback Method
tf	501.61	K	Joback Method
vc	0.956	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.00	J/molxK	755.57	Joback Method
cpg	710.02	J/molxK	785.62	Joback Method
cpg	722.28	J/molxK	815.66	Joback Method
cpg	733.79	J/molxK	845.71	Joback Method
cpg	744.56	J/molxK	875.76	Joback Method
cpg	754.60	J/molxK	905.81	Joback Method
cpg	763.93	J/molxK	935.85	Joback Method

# Sources

<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=U321546&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321546&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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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