

# Sebacic acid, octyl pentafluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C25H35F5O4/c1-2-3-4-5-10-13-16-33-19(31)14-11-8-6-7-9-12-15-20(32)34-17
<b>InchiKey:</b>	MLJCSDCUOCOTAZ-UHFFFAOYSA-N
<b>Formula:</b>	C25H35F5O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	494.54

## Physical Properties

Property code	Value	Unit	Source
gf	-1218.01	kJ/mol	Joback Method
hf	-1850.30	kJ/mol	Joback Method
hfus	73.58	kJ/mol	Joback Method
hvap	91.06	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	7.450		Crippen Method
mvol	363.080	ml/mol	McGowan Method
pc	818.66	kPa	Joback Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook
tb	971.91	K	Joback Method
tc	1200.48	K	Joback Method
tf	607.80	K	Joback Method
vc	1.466	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.15	J/molxK	971.91	Joback Method
cpg	1230.03	J/molxK	1010.01	Joback Method
cpg	1245.20	J/molxK	1048.10	Joback Method
cpg	1258.69	J/molxK	1086.20	Joback Method
cpg	1270.52	J/molxK	1124.29	Joback Method
cpg	1280.73	J/molxK	1162.39	Joback Method
cpg	1289.35	J/molxK	1200.48	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354903&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354903&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>

# 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>hvp:</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>rinp:</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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