

# Diglycolic acid, nonyl pentafluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C20H25F5O5/c1-2-3-4-5-6-7-8-9-29-14(26)11-28-12-15(27)30-10-13-16(21)18
<b>InchiKey:</b>	CQPSXANIAHYQJB-UHFFFAOYSA-N
<b>Formula:</b>	C20H25F5O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	440.40

## Physical Properties

Property code	Value	Unit	Source
gf	-1365.11	kJ/mol	Joback Method
hf	-1879.32	kJ/mol	Joback Method
hfus	61.81	kJ/mol	Joback Method
hvap	82.34	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	4.736		Crippen Method
mcvol	298.500	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpola	2933.00		NIST Webbook
rinpola	2933.00		NIST Webbook
tb	879.93	K	Joback Method
tc	1077.35	K	Joback Method
tf	573.68	K	Joback Method
vc	1.204	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.32	J/mol×K	879.93	Joback Method
cpg	954.49	J/mol×K	912.83	Joback Method
cpg	967.48	J/mol×K	945.74	Joback Method
cpg	979.28	J/mol×K	978.64	Joback Method
cpg	989.90	J/mol×K	1011.54	Joback Method
cpg	999.32	J/mol×K	1044.45	Joback Method
cpg	1007.53	J/mol×K	1077.35	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382078&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382078&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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