

# Diethylmalonic acid, octyl pentafluorobenzyl ester

Inchi:	InChI=1S/C22H29F5O4/c1-4-7-8-9-10-11-12-30-20(28)22(5-2,6-3)21(29)31-13-14-15(23
InchiKey:	RQYRMSRHYHJVHT-UHFFFAOYSA-N
Formula:	C22H29F5O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	452.46

## Physical Properties

Property code	Value	Unit	Source
gf	-1240.43	kJ/mol	Joback Method
hf	-1797.13	kJ/mol	Joback Method
hfus	58.39	kJ/mol	Joback Method
hvap	83.08	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	6.135		Crippen Method
mvol	320.810	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2159.00		NIST Webbook
rinpol	2159.00		NIST Webbook
tb	900.04	K	Joback Method
tc	1101.96	K	Joback Method
tf	576.41	K	Joback Method
vc	1.286	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.98	J/molxK	900.04	Joback Method
cpg	1046.09	J/molxK	933.69	Joback Method
cpg	1060.03	J/molxK	967.35	Joback Method
cpg	1072.82	J/molxK	1001.00	Joback Method
cpg	1084.51	J/molxK	1034.65	Joback Method
cpg	1095.10	J/molxK	1068.30	Joback Method
cpg	1104.64	J/molxK	1101.96	Joback Method

# Sources

<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=U369994&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369994&amp;Units=SI</a>
<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>

# 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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