

# Diethylmalonic acid, decyl 2,2,3,3,3-pentafluoropropyl ester

Inchi:	InChI=1S/C20H33F5O4/c1-4-7-8-9-10-11-12-13-14-28-16(26)18(5-2,6-3)17(27)29-15-19
InchiKey:	SQKSRLOBDGGEJW-UHFFFAOYSA-N
Formula:	C20H33F5O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)F
Mol. weight [g/mol]:	432.47

## Physical Properties

Property code	Value	Unit	Source
gf	-1315.85	kJ/mol	Joback Method
hf	-1952.53	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	70.45	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.218		Crippen Method
mvol	316.390	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	796.24	K	Joback Method
tc	975.77	K	Joback Method
tf	469.69	K	Joback Method
vc	1.260	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.70	J/mol×K	796.24	Joback Method
cpg	1026.45	J/mol×K	826.16	Joback Method
cpg	1042.21	J/mol×K	856.08	Joback Method
cpg	1057.04	J/mol×K	886.01	Joback Method
cpg	1070.99	J/mol×K	915.93	Joback Method
cpg	1084.11	J/mol×K	945.85	Joback Method
cpg	1096.46	J/mol×K	975.77	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=U370847&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370847&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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