

# Glutaric acid, octyl 2,3,4,5-tetrafluorobenzyl ester

Inchi:	InChI=1S/C20H26F4O4/c1-2-3-4-5-6-7-11-27-16(25)9-8-10-17(26)28-13-14-12-15(21)19
InchiKey:	BKWJNIZAMVGNCP-UHFFFAOYSA-N
Formula:	C20H26F4O4
SMILES:	CCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]:	406.41

## Physical Properties

Property code	Value	Unit	Source
gf	-1055.67	kJ/mol	Joback Method
hf	-1539.52	kJ/mol	Joback Method
hfus	57.93	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.360		Crippen Method
mvol	290.860	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	853.26	K	Joback Method
tc	1045.55	K	Joback Method
tf	538.34	K	Joback Method
vc	1.167	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.06	J/molxK	853.26	Joback Method
cpg	919.73	J/molxK	885.31	Joback Method
cpg	933.37	J/molxK	917.36	Joback Method
cpg	945.97	J/molxK	949.40	Joback Method
cpg	957.54	J/molxK	981.45	Joback Method
cpg	968.11	J/molxK	1013.50	Joback Method
cpg	977.67	J/molxK	1045.55	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=U377446&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377446&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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