

# Glutaric acid, 2,5-difluorobenzyl tetradecyl ester

Inchi:	InChI=1S/C26H40F2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-31-25(29)15-14-16-26(30)32
InchiKey:	ABQLNGYMCDBGHH-UHFFFAOYSA-N
Formula:	C26H40F2O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]:	454.59

## Physical Properties

Property code	Value	Unit	Source
gf	-596.27	kJ/mol	Joback Method
hf	-1248.20	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	93.75	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.423		Crippen Method
mcvol	371.860	ml/mol	McGowan Method
pc	859.48	kPa	Joback Method
rinpola	3053.00		NIST Webbook
rinpola	3053.00		NIST Webbook
tb	982.04	K	Joback Method
tc	1206.32	K	Joback Method
tf	579.74	K	Joback Method
vc	1.468	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.69	J/molxK	982.04	Joback Method
cpg	1274.12	J/molxK	1019.42	Joback Method
cpg	1289.93	J/molxK	1056.80	Joback Method
cpg	1304.17	J/molxK	1094.18	Joback Method
cpg	1316.89	J/molxK	1131.56	Joback Method
cpg	1328.14	J/molxK	1168.94	Joback Method
cpg	1337.96	J/molxK	1206.32	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.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>
<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=U376956&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376956&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>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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