

# Glutaric acid, 2-fluoro-6-(trifluoromethyl)benzyl heptyl ester

Inchi:	InChI=1S/C20H26F4O4/c1-2-3-4-5-6-13-27-18(25)11-8-12-19(26)28-14-15-16(20(22,23)
InchiKey:	HFAYFVLGICXNHP-UHFFFAOYSA-N
Formula:	C20H26F4O4
SMILES:	CCCCCCCOC(=O)CCCC(=O)OCc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]:	406.41

## Physical Properties

Property code	Value	Unit	Source
gf	-1033.57	kJ/mol	Joback Method
hf	-1525.33	kJ/mol	Joback Method
hfus	51.30	kJ/mol	Joback Method
hvap	77.46	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.572		Crippen Method
mcvol	290.860	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinqol	2527.00		NIST Webbook
tb	840.07	K	Joback Method
tc	1031.79	K	Joback Method
tf	515.72	K	Joback Method
vc	1.157	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.57	J/molxK	840.07	Joback Method
cpg	922.28	J/molxK	872.02	Joback Method
cpg	935.97	J/molxK	903.98	Joback Method
cpg	948.67	J/molxK	935.93	Joback Method
cpg	960.43	J/molxK	967.89	Joback Method
cpg	971.28	J/molxK	999.84	Joback Method
cpg	981.24	J/molxK	1031.79	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=U377503&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377503&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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