

# Glutaric acid, 4-cyanophenyl hexyl ester

<b>Inchi:</b>	InChI=1S/C18H23NO4/c1-2-3-4-5-13-22-17(20)7-6-8-18(21)23-16-11-9-15(14-19)10-12-
<b>InchiKey:</b>	OZQOUUWTOCKVDS-UHFFFAOYSA-N
<b>Formula:</b>	C18H23NO4
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)Oc1ccc(C#N)cc1
<b>Mol. weight [g/mol]:</b>	317.38

## Physical Properties

Property code	Value	Unit	Source
gf	-131.20	kJ/mol	Joback Method
hf	-514.51	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	87.39	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.757		Crippen Method
mvol	256.980	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2561.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	897.56	K	Joback Method
tc	1111.56	K	Joback Method
tf	540.87	K	Joback Method
vc	1.010	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.92	J/mol×K	897.56	Joback Method
cpg	797.44	J/mol×K	933.23	Joback Method
cpg	808.85	J/mol×K	968.89	Joback Method
cpg	819.18	J/mol×K	1004.56	Joback Method
cpg	828.44	J/mol×K	1040.23	Joback Method
cpg	836.65	J/mol×K	1075.90	Joback Method
cpg	843.84	J/mol×K	1111.56	Joback Method

# Sources

<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=U358615&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358615&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>

# 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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