

# Glutaric acid, 8-chlorooctyl 4-cyanophenyl ester

Inchi:	InChI=1S/C20H26ClNO4/c21-14-5-3-1-2-4-6-15-25-19(23)8-7-9-20(24)26-18-12-10-17(1
InchiKey:	XKNVCOJOKRGADV-UHFFFAOYSA-N
Formula:	C20H26ClNO4
SMILES:	N#Cc1ccc(OC(=O)CCCC(=O)OCCCCCCCCCl)cc1
Mol. weight [g/mol]:	379.88

## Physical Properties

Property code	Value	Unit	Source
gf	-126.29	kJ/mol	Joback Method
hf	-571.53	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	96.23	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.757		Crippen Method
mvol	297.400	ml/mol	McGowan Method
pc	1282.83	kPa	Joback Method
rinpol	3086.00		NIST Webbook
tb	980.75	K	Joback Method
tc	1203.50	K	Joback Method
tf	593.33	K	Joback Method
vc	1.171	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.14	J/mol×K	980.75	Joback Method
cpg	934.86	J/mol×K	1017.88	Joback Method
cpg	945.36	J/mol×K	1055.00	Joback Method
cpg	954.66	J/mol×K	1092.13	Joback Method
cpg	962.79	J/mol×K	1129.25	Joback Method
cpg	969.79	J/mol×K	1166.38	Joback Method
cpg	975.68	J/mol×K	1203.50	Joback Method

# Sources

<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.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>
<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=U393281&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393281&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>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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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