

# Glutaric acid, hept-2-yl 4-cyanophenyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H25NO4/c1-3-4-5-7-15(2)23-18(21)8-6-9-19(22)24-17-12-10-16(14-20)11-

DAZRCVWSJIFVFU-UHFFFAOYSA-N

C19H25NO4

CCCCC(C)OC(=O)CCCC(=O)Oc1ccc(C#N)cc1

331.41

## Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-540.43	kJ/mol	Joback Method
hfus	42.17	kJ/mol	Joback Method
hvap	89.23	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.146		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	2518.00		NIST Webbook
tb	920.00	K	Joback Method
tc	1136.39	K	Joback Method
tf	537.14	K	Joback Method
vc	1.060	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.30	J/molxK	920.00	Joback Method
cpg	856.08	J/molxK	956.06	Joback Method
cpg	867.67	J/molxK	992.13	Joback Method
cpg	878.11	J/molxK	1028.19	Joback Method
cpg	887.40	J/molxK	1064.26	Joback Method
cpg	895.59	J/molxK	1100.32	Joback Method
cpg	902.68	J/molxK	1136.39	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393274&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393274&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mcvol:</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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