

# Glycerol tribenzoate

<b>Inchi:</b>	InChI=1S/C24H20O6/c25-22(28-19-12-6-2-7-13-19)16-21(30-24(27)18-10-4-1-5-11-18)1
<b>InchiKey:</b>	CEIXSUMKBRIAAH-UHFFFAOYSA-N
<b>Formula:</b>	C24H20O6
<b>SMILES:</b>	O=C(CC(CC(=O)Oc1ccccc1)OC(=O)c1ccccc1)Oc1ccccc1
<b>Mol. weight [g/mol]:</b>	404.41

## Physical Properties

Property code	Value	Unit	Source
gf	-215.77	kJ/mol	Joback Method
hf	-568.78	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	102.93	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.203		Crippen Method
mcvol	300.060	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
tb	1056.99	K	Joback Method
tc	1309.45	K	Joback Method
tf	640.98	K	Joback Method
vc	1.121	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.18	J/molxK	1056.99	Joback Method
cpg	965.48	J/molxK	1267.37	Joback Method
cpg	963.23	J/molxK	1225.30	Joback Method
cpg	959.55	J/molxK	1183.22	Joback Method
cpg	954.36	J/molxK	1141.14	Joback Method
cpg	947.60	J/molxK	1099.07	Joback Method
cpg	966.36	J/molxK	1309.45	Joback Method
dvisc	0.0000203	Paxs	1056.99	Joback Method
dvisc	0.0000261	Paxs	987.65	Joback Method
dvisc	0.0000350	Paxs	918.32	Joback Method

dvisc	0.0000491	Paxs	848.99	Joback Method
dvisc	0.0000732	Paxs	779.65	Joback Method
dvisc	0.0001181	Paxs	710.32	Joback Method
dvisc	0.0002110	Paxs	640.98	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001721&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001721&amp;Units=SI</a>
<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.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>dvisc:</b>	Dynamic viscosity
<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>hvac:</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>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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