

Glycerol tribenzoate

Inchi:

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

InchiKey:

CEIXSUMKBRIAAH-UHFFFAOYSA-N

Formula:

C24H20O6

SMILES:

O=C(CC(CC(=O)Oc1ccccc1)OC(=O)c1ccccc1)Oc1ccccc1

Mol. weight [g/mol]:

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/mol×K	1056.99	Joback Method
cpg	965.48	J/mol×K	1267.37	Joback Method
cpg	963.23	J/mol×K	1225.30	Joback Method
cpg	959.55	J/mol×K	1183.22	Joback Method
cpg	954.36	J/mol×K	1141.14	Joback Method
cpg	947.60	J/mol×K	1099.07	Joback Method
cpg	966.36	J/mol×K	1309.45	Joback Method
dvisc	0.0000203	Pa×s	1056.99	Joback Method
dvisc	0.0000261	Pa×s	987.65	Joback Method
dvisc	0.0000350	Pa×s	918.32	Joback Method

dvisc	0.0000491	Pa×s	848.99	Joback Method
dvisc	0.0000732	Pa×s	779.65	Joback Method
dvisc	0.0001181	Pa×s	710.32	Joback Method
dvisc	0.0002110	Pa×s	640.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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