

4,4',4''-Trimethyltrityl alcohol

Other names:

Benzenemethanol, 4-methyl-«alpha», «alpha»-bis(4-methylphenyl)-
Methanol, tri-p-tolyl-
Tri(p-tolyl)methanol
Tris(4-methylphenyl)methanol
4,4',4''-Trimethyltriphenylmethanol
4,4',4''-trimethyltrityl alcohol

Inchi:

InChI=1S/C22H22O/c1-16-4-10-19(11-5-16)22(23,20-12-6-17(2)7-13-20)21-14-8-18(3)9-

InchiKey:

DNWQXZDDISHGRM-UHFFFAOYSA-N

Formula:

C22H22O

SMILES:

Cc1ccc(C(O)(c2ccc(C)cc2)c2ccc(C)cc2)cc1

Mol. weight [g/mol]:

302.41

CAS:

3247-00-5

Physical Properties

Property code	Value	Unit	Source
gf	308.72	kJ/mol	Joback Method
hf	16.79	kJ/mol	Joback Method
hfs	-67.00 ± 24.00	kJ/mol	NIST Webbook
hfus	30.37	kJ/mol	Joback Method
hvap	88.76	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.896		Crippen Method
mcvol	255.430	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
tb	886.69	K	Joback Method
tc	1127.94	K	Joback Method
tf	364.65 ± 2.00	K	NIST Webbook
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.27	J/mol×K	886.69	Joback Method
cpg	834.75	J/mol×K	1087.74	Joback Method

cpg	823.72	J/molxK	1047.53	Joback Method
cpg	811.99	J/molxK	1007.32	Joback Method
cpg	799.43	J/molxK	967.11	Joback Method
cpg	785.90	J/molxK	926.90	Joback Method
cpg	845.20	J/molxK	1127.94	Joback Method
dvisc	0.0000100	Paxs	886.69	Joback Method
dvisc	0.0000143	Paxs	825.20	Joback Method
dvisc	0.0000218	Paxs	763.71	Joback Method
dvisc	0.0000356	Paxs	702.23	Joback Method
dvisc	0.0000640	Paxs	640.74	Joback Method
dvisc	0.0001303	Paxs	579.25	Joback Method
dvisc	0.0003140	Paxs	517.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3247005&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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