

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]:	302.42

Physical Properties

Property code	Value	Unit	Source
af	0.8092		Cheméo Relay (1.0)
gf	308.72	kJ/mol	Joback Method
hf	37.94	kJ/mol	Cheméo Relay (1.0)
hfs	-67.00 ± 24.00	kJ/mol	NIST Webbook
hfus	30.37	kJ/mol	Joback Method
hvap	109.80	kJ/mol	Cheméo Relay (1.0)
ie	8.06	eV	Cheméo Relay (1.0)
log10ws	-4.95		Cheméo Relay (1.0)
logp	4.896		Crippen Method
mcvol	255.430	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
tb	644.78	K	Cheméo Relay (1.0)
tc	973.67	K	Cheméo Relay (1.0)
tf	364.65 ± 2.00	K	NIST Webbook
vc	0.924	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	785.90	J/mol×K	926.90	Joback Method
cpg	799.43	J/mol×K	967.11	Joback Method
cpg	811.99	J/mol×K	1007.32	Joback Method
cpg	823.72	J/mol×K	1047.53	Joback Method
cpg	834.75	J/mol×K	1087.74	Joback Method
cpg	845.20	J/mol×K	1127.94	Joback Method
dvisc	0.0003140	Pa×s	517.76	Joback Method
dvisc	0.0001303	Pa×s	579.25	Joback Method
dvisc	0.0000640	Pa×s	640.74	Joback Method
dvisc	0.0000356	Pa×s	702.23	Joback Method
dvisc	0.0000218	Pa×s	763.71	Joback Method
dvisc	0.0000143	Pa×s	825.20	Joback Method
dvisc	0.0000100	Pa×s	886.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3247005&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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