

Ethenol, 2,2-bis(2,4,6-trimethylphenyl)-

Inchi:	InChI=1S/C20H24O/c1-12-7-14(3)19(15(4)8-12)18(11-21)20-16(5)9-13(2)10-17(20)6/h7-
InchiKey:	ZEWSRGXZSLAREL-UHFFFAOYSA-N
Formula:	C20H24O
SMILES:	<chem>Cc1cc(C)c(C(=CO)c2c(C)cc(C)cc2C)c(C)c1</chem>
Mol. weight [g/mol]:	280.40
CAS:	54288-04-9

Physical Properties

Property code	Value	Unit	Source
gf	219.41	kJ/mol	Joback Method
hf	-96.69	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Joback Method
hvap	85.36	kJ/mol	Joback Method
ie	7.60 ± 0.05	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
log10ws	-6.68		Crippen Method
logp	5.484		Crippen Method
mcvol	246.710	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
tb	836.46	K	Joback Method
tc	1053.87	K	Joback Method
tf	484.90	K	Joback Method
vc	0.940	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.49	J/mol×K	836.46	Joback Method
cpg	737.58	J/mol×K	872.70	Joback Method
cpg	751.76	J/mol×K	908.93	Joback Method
cpg	765.06	J/mol×K	945.17	Joback Method
cpg	777.56	J/mol×K	981.40	Joback Method
cpg	789.29	J/mol×K	1017.64	Joback Method
cpg	800.32	J/mol×K	1053.87	Joback Method

Sources

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=C54288049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
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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