1-Propen-2-ol, 1,1-bis(2,4,6-trimethylphenyl)-

Inchi: InChI=1S/C21H26O/c1-12-8-14(3)19(15(4)9-12)21(18(7)22)20-16(5)10-13(2)11-17(20)6/
InchiKey: UIXTVSOEEDOJBG-UHFFFAOYSA-N
Formula: C21H26O
SMILES: CC(O)=C(c1c(C)cc(C)cc1C)c1c(C)cc(C)cc1C
Mol. weight [g/mol]: 294.43
CAS: 89959-15-9

Physical Properties

Property code	Value	Unit	Source
gf	219.28	kJ/mol	Joback Method
hf	-127.12	kJ/mol	Joback Method
hfus	37.56	kJ/mol	Joback Method
hvap	87.66	kJ/mol	Joback Method
ie	7.50 ± 0.05	eV	NIST Webbook
log10ws	-7.10		Crippen Method
logp	5.874		Crippen Method
mcvol	260.800	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
tb	859.22	K	Joback Method
tc	1077.45	K	Joback Method
tf	482.21	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.87	J/mol×K	859.22	Joback Method
cpg	795.42	J/mol×K	895.59	Joback Method
cpg	810.02	J/mol×K	931.96	Joback Method
cpg	823.73	J/mol×K	968.33	Joback Method
cpg	836.61	J/mol×K	1004.71	Joback Method
cpg	848.73	J/mol×K	1041.08	Joback Method
cpg	860.13	J/mol×K	1077.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89959159&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
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