1,7-Octadiene-3,6-diol, 2,6-dimethyl-

Other names:	2,6-Dimethyl-1,7-octadien-3,6-diol
	2,6-Dimethyl-octa-1,7-dien-3,6-diol
	3,7-Dimethyl-1,7-octadien-3,6-diol
	3,7-Dimethyl-1,7-octadiene-3,6-diol
	3,7-Dimethylocta-1,7-dien-3,6-diol
	3,7-Dimethylocta-1,7-diene-3,6-diol
	2,6-Dimethylocta-1,7-diene-3,6-diol
	2,6-Dimethyl-1,7-octadiene-3,6-diol
Inchi:	InChI=1S/C10H18O2/c1-5-10(4,12)7-6-9(11)8(2)3/h5,9,11-12H,1-2,6-7H2,3-4H3
InchiKey:	HZHJGFRDKJPQPV-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CC(C)(O)CCC(O)C(=C)C
Mol. weight [g/mol]:	170.25
CAS:	51276-33-6

Physical Properties

Property code	Value	Unit	Source
gf	-72.79	kJ/mol	Joback Method
hf	-327.15	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	68.27	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.641		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2128.00		NIST Webbook

ripol	2134.00		NIST Webbook
ripol	2136.00		NIST Webbook
ripol	2128.00		NIST Webbook
ripol	2128.00		NIST Webbook
ripol	2128.00		NIST Webbook
tb	602.13	K	Joback Method
tc	774.34	K	Joback Method
tf	294.04	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.84	J/mol×K	602.13	Joback Method
cpg	414.05	J/mol×K	630.83	Joback Method
cpg	424.67	J/mol×K	659.53	Joback Method
cpg	434.72	J/mol×K	688.24	Joback Method
cpg	444.26	J/mol×K	716.94	Joback Method
cpg	453.30	J/mol×K	745.64	Joback Method
cpg	461.89	J/mol×K	774.34	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51276336&Units=SI

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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume