2,7-Octadien-4-ol, 2-methyl-6-methylene-, (S)-

Other names:	2-Methyl-6-methylene-2,7-octadien-4-ol
	Ipsdienol
	2,7-Octadien-4-ol, 2-methyl-6-methylene-, (4S)-
Inchi:	InChI=1S/C10H16O/c1-5-9(4)7-10(11)6-8(2)3/h5-6,10-11H,1,4,7H2,2-3H3
InchiKey:	NHMKYUHMPXBMFI-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	C=CC(=C)CC(O)C=C(C)C
Mol. weight [g/mol]:	152.23
CAS:	35628-00-3

Physical Properties

Property code	Value	Unit	Source
gf	132.86	kJ/mol	Joback Method
hf	-58.74	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.446		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1129.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1147.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1678.00		NIST Webbook

ripol	1584.00		NIST Webbook
tb	517.22	K	Joback Method
tc	696.85	K	Joback Method
tf	211.76	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.42	J/mol×K	517.22	Joback Method
cpg	337.80	J/mol×K	547.16	Joback Method
cpg	349.55	J/mol×K	577.10	Joback Method
cpg	360.70	J/mol×K	607.04	Joback Method
cpg	371.27	J/mol×K	636.98	Joback Method
cpg	381.31	J/mol×K	666.91	Joback Method
cpg	390.84	J/mol×K	696.85	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35628003&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

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