2,3-Dehydro-1,4-cineol

Other names: p-Menth-2-ene, 1,4-epoxy
Inchi: InChI=1S/C10H16O/c1-8(2)10-6-4-9(3,11-10)5-7-10/h4,6,8H,5,7H2,1-3H3
InchiKey: KSMRNKXOGJCMES-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC(C)C12C=CC(C)(CC1)O2
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	73.14	kJ/mol	Joback Method
hf	-159.31	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	39.96	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.520		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
tb	472.10	K	Joback Method
tc	693.76	K	Joback Method
tf	294.95	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.77	J/mol×K	472.10	Joback Method
cpg	323.66	J/mol×K	509.04	Joback Method
cpg	339.83	J/mol×K	545.99	Joback Method
cpg	354.54	J/mol×K	582.93	Joback Method
cpg	368.05	J/mol×K	619.87	Joback Method
cpg	380.62	J/mol×K	656.81	Joback Method
cpg	392.52	J/mol×K	693.76	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=R425257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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