

2,3-Dehydro-1,8-cineole

Other names:	1,8-Dehydro-cineole
Inchi:	InChI=1S/C10H16O/c1-9(2)8-4-6-10(3,11-9)7-5-8/h4,6,8H,5,7H2,1-3H3
InchiKey:	LOOYOTLEOHYYOV-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC12C=CC(CC1)C(C)(C)O2
Mol. weight [g/mol]:	152.23
CAS:	92760-25-3

Physical Properties

Property code	Value	Unit	Source
gf	55.77	kJ/mol	Joback Method
hf	-180.53	kJ/mol	Joback Method
hfus	11.40	kJ/mol	Joback Method
hvap	40.22	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.520		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	979.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	994.00		NIST Webbook
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rinpol	994.00		NIST Webbook
rinpol	993.00		NIST Webbook
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rinpol	975.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	994.70		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	988.00		NIST Webbook

rinpol	991.00	NIST Webbook
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rinpol	991.00	NIST Webbook
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ripol	1197.00	NIST Webbook
ripol	1195.00	NIST Webbook
ripol	1195.00	NIST Webbook
ripol	1195.00	NIST Webbook

tb	472.14	K	Joback Method
tc	697.01	K	Joback Method
tf	302.19	K	Joback Method
vc	0.495	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.81	J/mol×K	472.14	Joback Method
cpg	324.67	J/mol×K	509.62	Joback Method
cpg	341.81	J/mol×K	547.10	Joback Method
cpg	357.49	J/mol×K	584.58	Joback Method
cpg	371.95	J/mol×K	622.05	Joback Method
cpg	385.46	J/mol×K	659.53	Joback Method
cpg	398.28	J/mol×K	697.01	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=C92760253&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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