3,4-Dehydrocineole

Inchi: InChI=1S/C10H16O/c1-9(2)8-4-6-10(3,11-9)7-5-8/h4H,5-7H2,1-3H3
InchiKey: CAEVFYKCVGNSKS-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC12CC=C(CC1)C(C)(C)O2
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	53.85	kJ/mol	Joback Method
hf	-171.66	kJ/mol	Joback Method
hfus	9.94	kJ/mol	Joback Method
hvap	41.19	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.664		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1197.00		NIST Webbook
tb	481.79	K	Joback Method
tc	708.23	K	Joback Method
tf	318.95	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.37	J/mol×K	481.79	Joback Method
cpg	324.18	J/mol×K	519.53	Joback Method
cpg	340.36	J/mol×K	557.27	Joback Method
cpg	355.16	J/mol×K	595.01	Joback Method
cpg	368.87	J/mol×K	632.75	Joback Method
cpg	381.73	J/mol×K	670.49	Joback Method

cpg	394.01	J/mol×K	708.23	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=R285608&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