2«alpha»,9-dihydroxy-1,8-cineole

Inchi: InChI=1S/C10H18O3/c1-9-4-3-7(5-8(9)12)10(2,6-11)13-9/h7-8,11-12H,3-6H2,1-2H3/t7?,
InchiKey: YBBFHZOLGNSKEP-CFEUDACVSA-N
Formula: C10H18O3
SMILES: CC12CCC(CC1O)C(C)(CO)O2
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
gf	-255.54	kJ/mol	Joback Method
hf	-563.11	kJ/mol	Joback Method
hfus	19.43	kJ/mol	Joback Method
hvap	72.97	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	0.687		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
ripol	2801.00		NIST Webbook
ripol	2801.00		NIST Webbook
tb	652.67	K	Joback Method
tc	846.80	K	Joback Method
tf	418.83	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.14	J/mol×K	652.67	Joback Method
cpg	457.14	J/mol×K	685.02	Joback Method
cpg	469.66	J/mol×K	717.38	Joback Method
cpg	481.86	J/mol×K	749.73	Joback Method
cpg	493.90	J/mol×K	782.09	Joback Method
cpg	505.94	J/mol×K	814.44	Joback Method
cpg	518.15	J/mol×K	846.80	Joback Method

Sources

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=R404161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume