Exo-2-hydroxycineole

Other names: 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octan-6-ol, (1«alpha»,4«alpha»,6«beta»)-
2-Hydroxycineole, exo-
2-exo-Hydroxy-1,8-cineole
2«alpha»-Hydroxy-1,8-cineol
2«alpha»-Hydroxy-1,8-cineole
exo-2-Hydroxy-8-cineole
exo-2-Hydroxycineol
trans-2-Hydroxy-1,8-cineole

Inchi: InChI=1S/C10H18O2/c1-9(2)7-4-5-10(3,12-9)8(11)6-7/h7-8,11H,4-6H2,1-3H3/t7?,8-,10?/

InchiKey: YVCUGZBVCHODNB-ZCUBBSJVSA-N

Formula: C10H18O2

SMILES: CC1(C)OC2(C)CCC1C[C@H]2O

Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
hfus	15.34	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Cheméo Relay (1.0)
log10ws	-1.37		Cheméo Relay (1.0)
logp	1.715		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
rinpol	1219.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1230.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1859.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1888.00		NIST Webbook
ripol	1861.00		NIST Webbook

ripol	1845.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1834.00		NIST Webbook
tb	505.87	K	Cheméo Relay (1.0)
tf	391.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.49	J/mol×K	560.49	Joback Method
cpg	402.41	J/mol×K	594.92	Joback Method
cpg	417.30	J/mol×K	629.36	Joback Method
cpg	431.35	J/mol×K	663.79	Joback Method
cpg	444.77	J/mol×K	698.23	Joback Method
cpg	457.73	J/mol×K	732.66	Joback Method
cpg	470.44	J/mol×K	767.10	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92999785&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point