Bicyclo[3.1.1]heptan-3-ol, 2,6,6-trimethyl-, (1«alpha»,2«beta»,3«alpha»,5«alpha»)-

Other names: 3-Pinanol, stereoisomer
Isopinocampheol
2,6,6-Trimethylbicyclo[3.1.1]heptan-3-ol-, (1R,2R,3R,5S)-rel-
(1«alpha»,2«beta»,3«alpha»,5«alpha»)-2,6,6-trimethylbicyclo[3.1.1]heptan-3-ol

Inchi: InChI=1S/C10H18O/c1-6-8-4-7(5-9(6)11)10(8,2)3/h6-9,11H,4-5H2,1-3H3

InchiKey: REPVLJRCJUVQFA-UHFFFAOYSA-N

Formula: C10H18O

SMILES: CC1C(O)CC2CC1C2(C)C

Mol. weight [g/mol]: 154.25

CAS: 27779-29-9

Physical Properties

Property code	Value	Unit	Source
gf	-22.72	kJ/mol	Joback Method
hf	-308.30	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	52.45	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.049		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1168.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1120.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1703.00		NIST Webbook
tb	492.20	K	NIST Webbook
tc	717.42	K	Joback Method

tf	306.82	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.48	J/mol×K	524.36	Joback Method
cpg	372.00	J/mol×K	556.54	Joback Method
cpg	387.53	J/mol×K	588.71	Joback Method
cpg	402.17	J/mol×K	620.89	Joback Method
cpg	416.03	J/mol×K	653.07	Joback Method
cpg	429.20	J/mol×K	685.24	Joback Method
cpg	441.78	J/mol×K	717.42	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27779299&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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