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

Other names: (+)-Isopinocampheol
[1S-(1«alpha»,2«beta»,3«alpha»,5«alpha»)]-2,6,6-trimethylbicyclo[3.1.1]heptan-3-ol
Inchi: InChI=1S/C12H22O/c1-8-9(13)6-11(4)7-12(8,5)10(11,2)3/h8-9,13H,6-7H2,1-5H3/t8-,9+,1
InchiKey: NJBQFUAXCUCPGX-LUTQBAROSA-N
Formula: C10H18O
SMILES: CC1C(O)CC2(C)CC1(C)C2(C)C
Mol. weight [g/mol]: 154.25
CAS: 24041-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-16.86	kJ/mol	Joback Method
hf	-182.00 ± 8.40	kJ/mol	NIST Webbook
hfus	9.41	kJ/mol	Joback Method
hvap	54.60	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.830		Crippen Method
mcvol	164.090	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	570.60	K	Joback Method
tc	773.27	K	Joback Method
tf	377.16	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.56	J/mol×K	570.60	Joback Method
cpg	468.65	J/mol×K	604.38	Joback Method
cpg	484.71	J/mol×K	638.16	Joback Method
cpg	499.98	J/mol×K	671.94	Joback Method
cpg	514.73	J/mol×K	705.72	Joback Method
cpg	529.22	J/mol×K	739.50	Joback Method
cpg	543.70	J/mol×K	773.27	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=C24041609&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume