Menthane, 1,2,4-trihydroxy

Inchi: InChI=1S/C10H20O3/c1-7(2)10(13)5-4-9(3,12)8(11)6-10/h7-8,11-13H,4-6H2,1-3H3/t8-,9
InchiKey: RKROZYQLIWCOBD-OPRDCNLKSA-N
Formula: C10H20O3
SMILES: CC(C)C1(O)CCC(C)(O)C(O)C1
Mol. weight [g/mol]: 188.26
CAS: 22555-61-9

Physical Properties

Property code	Value	Unit	Source
gf	-381.53	kJ/mol	Joback Method
hf	-667.58	kJ/mol	Joback Method
hfus	11.78	kJ/mol	Joback Method
hvap	85.01	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	0.669		Crippen Method
mcvol	158.510	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1486.70		NIST Webbook
rinpol	1486.70		NIST Webbook
tb	714.99	K	Joback Method
tc	900.45	K	Joback Method
tf	416.62	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.45	J/mol×K	714.99	Joback Method
cpg	499.88	J/mol×K	745.90	Joback Method
cpg	512.10	J/mol×K	776.81	Joback Method
cpg	524.21	J/mol×K	807.72	Joback Method
cpg	536.35	J/mol×K	838.63	Joback Method

cpg	548.63	J/mol×K	869.54	Joback Method
cpg	561.18	J/mol×K	900.45	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=C22555619&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume