2,2-dimethylcyclohexanol

Inchi: InChI=1S/C8H16O/c1-8(2)6-4-3-5-7(8)9/h7,9H,3-6H2,1-2H3
InchiKey: BYBYZPFVXFPCND-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CC1(C)CCCCC1O
Mol. weight [g/mol]: 128.21
CAS: 1193-46-0

Physical Properties

Property code	Value	Unit	Source
hfus	7.17	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Cheméo Relay (1.0)
logp	1.948		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
tb	450.24	K	Cheméo Relay (1.0)
tf	339.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.75	J/mol×K	489.74	Joback Method
cpg	290.94	J/mol×K	522.76	Joback Method
cpg	305.22	J/mol×K	555.79	Joback Method
cpg	318.68	J/mol×K	588.81	Joback Method
cpg	331.39	J/mol×K	621.83	Joback Method
cpg	343.44	J/mol×K	654.85	Joback Method
cpg	354.91	J/mol×K	687.88	Joback Method

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50547e+01
Coeff. B	-4.11748e+03
Coeff. C	-6.62920e+01
Temperature range (K), min.	345.12
Temperature range (K), max.	488.89

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pvap: Vapor pressure
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point