TRICYCLO[3.3.1.1(3,7)]DECANE-2,6-DIOL

Other names: 2,6-Dihydroxyadamantane
Inchi: InChI=1S/C10H16O2/c11-9-5-1-6-3-8(9)4-7(2-5)10(6)12/h5-12H,1-4H2
InchiKey: MJHGVORZDBZFTH-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: OC1C2CC3CC1CC(C2)C3O
Mol. weight [g/mol]: 168.24

Physical Properties

Property code	Value	Unit	Source
hf	-396.84	kJ/mol	Cheméo Relay (1.0)
hfus	25.35	kJ/mol	Joback Method
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-2.49		Cheméo Relay (1.0)
logp	0.774		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
rinpol	1625.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	546.18	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.24	J/mol×K	623.04	Joback Method
cpg	419.41	J/mol×K	654.42	Joback Method
cpg	432.75	J/mol×K	685.80	Joback Method
cpg	445.32	J/mol×K	717.19	Joback Method
cpg	457.18	J/mol×K	748.57	Joback Method
cpg	468.39	J/mol×K	779.95	Joback Method
cpg	479.01	J/mol×K	811.33	Joback Method
dvisc	0.0095688	Pa×s	361.68	Joback Method

dvisc	0.0044001	Pa×s	405.24	Joback Method
dvisc	0.0023527	Pa×s	448.80	Joback Method
dvisc	0.0014053	Pa×s	492.36	Joback Method
dvisc	0.0009128	Pa×s	535.92	Joback Method
dvisc	0.0006326	Pa×s	579.48	Joback Method
dvisc	0.0004615	Pa×s	623.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25106972&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):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature