

Tricyclo[3.3.1.1(3,7)]decane-2,4-diol

Other names:	2(e),4(a)-Dihydroxyadamantane
Inchi:	InChI=1S/C10H16O2/c11-9-6-1-5-2-7(4-6)10(12)8(9)3-5/h5-12H,1-4H2
InchiKey:	PBWYCJIFRBPVPW-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	OC1C2CC3CC(C2)C(O)C1C3
Mol. weight [g/mol]:	168.23
CAS:	19213-99-1

Physical Properties

Property code	Value	Unit	Source
gf	-93.30	kJ/mol	Joback Method
hf	-402.97	kJ/mol	Joback Method
hfus	25.35	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	0.774		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	623.04	K	Joback Method
tc	811.33	K	Joback Method
tf	361.68	K	Joback Method
vc	0.493	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.24	J/molxK	623.04	Joback Method
cpg	468.39	J/molxK	779.95	Joback Method

cpg	457.18	J/molxK	748.57	Joback Method
cpg	445.32	J/molxK	717.19	Joback Method
cpg	432.75	J/molxK	685.80	Joback Method
cpg	419.41	J/molxK	654.42	Joback Method
cpg	479.01	J/molxK	811.33	Joback Method
dvisc	0.0004615	Paxs	623.04	Joback Method
dvisc	0.0006326	Paxs	579.48	Joback Method
dvisc	0.0009128	Paxs	535.92	Joback Method
dvisc	0.0014053	Paxs	492.36	Joback Method
dvisc	0.0023527	Paxs	448.80	Joback Method
dvisc	0.0044001	Paxs	405.24	Joback Method
dvisc	0.0095688	Paxs	361.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19213991&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
dvisc:	Dynamic viscosity
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

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