

Tricyclo[3.2.1.0^{2,4}]octan-8-ol,endo-anti-

Inchi:	InChI=1S/C8H12O/c9-8-4-1-2-5(8)7-3-6(4)7/h4-9H,1-3H2/t4?,5?,6-,7+,8?
InchiKey:	KKIDVQSXZVWGTL-GLXUGZOWSA-N
Formula:	C8H12O
SMILES:	OC1C2CCC1C1CC21
Mol. weight [g/mol]:	124.18
CAS:	16384-97-7

Physical Properties

Property code	Value	Unit	Source
gf	58.59	kJ/mol	Joback Method
hf	-176.80	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Joback Method
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-1.26		Crippen Method
logp	1.023		Crippen Method
mcvol	96.870	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
tb	481.23	K	Joback Method
tc	672.05	K	Joback Method
tf	289.60	K	Joback Method
vc	0.380	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.39	J/molxK	481.23	Joback Method
cpg	262.57	J/molxK	513.03	Joback Method
cpg	275.79	J/molxK	544.84	Joback Method
cpg	288.12	J/molxK	576.64	Joback Method
cpg	299.62	J/molxK	608.44	Joback Method
cpg	310.37	J/molxK	640.25	Joback Method
cpg	320.45	J/molxK	672.05	Joback Method
dvisc	0.0031626	Paxs	289.60	Joback Method

dvisc	0.0026396	Paxs	321.54	Joback Method
dvisc	0.0022763	Paxs	353.48	Joback Method
dvisc	0.0020117	Paxs	385.42	Joback Method
dvisc	0.0018118	Paxs	417.35	Joback Method
dvisc	0.0016563	Paxs	449.29	Joback Method
dvisc	0.0015322	Paxs	481.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C16384977&Units=SI

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
ie:	Ionization energy
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

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