

Trans-dihydroperillaldehyde

Other names:	trans-1,2-Dihydroperillaldehyde
Inchi:	InChI=1S/C10H16O/c1-8(2)10-5-3-9(7-11)4-6-10/h7,9-10H,1,3-6H2,2H3/t9-,10-
InchiKey:	AOVAKEPXE OVCEW-MGCOHNPYSA-N
Formula:	C10H16O
SMILES:	C=C(C)C1CCC(C=O)CC1
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	29.83	kJ/mol	Joback Method
hf	-185.69	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	44.10	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1180.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1174.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1606.00		NIST Webbook
tb	488.30	K	Joback Method
tc	698.48	K	Joback Method
tf	231.88	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.91	J/mol×K	488.30	Joback Method
cpg	328.95	J/mol×K	523.33	Joback Method
cpg	346.01	J/mol×K	558.36	Joback Method

cpg	362.13	J/mol×K	593.39	Joback Method
cpg	377.32	J/mol×K	628.42	Joback Method
cpg	391.62	J/mol×K	663.45	Joback Method
cpg	405.06	J/mol×K	698.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R196197&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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