

Perillic aldehyde

Inchi:	InChI=1S/C10H14O/c1-8(2)10-5-3-9(7-11)4-6-10/h3,7,10H,1,4-6H2,2H3/t10-/m1/s1
InchiKey:	RUMOYJJNUMEFDD-SNVBAGLBSA-N
Formula:	C10H14O
SMILES:	C=C(C)C1CC=C(C=O)CC1
Mol. weight [g/mol]:	150.22

Physical Properties

Property code	Value	Unit	Source
gf	57.87	kJ/mol	Joback Method
hf	-119.04	kJ/mol	Joback Method
hfus	14.02	kJ/mol	Joback Method
hvap	45.37	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
tb	497.11	K	Joback Method
tc	710.87	K	Joback Method
tf	249.40	K	Joback Method
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.38	J/mol×K	497.11	Joback Method
cpg	310.40	J/mol×K	532.74	Joback Method
cpg	325.51	J/mol×K	568.36	Joback Method
cpg	339.74	J/mol×K	603.99	Joback Method
cpg	353.13	J/mol×K	639.62	Joback Method
cpg	365.70	J/mol×K	675.25	Joback Method
cpg	377.49	J/mol×K	710.87	Joback Method

Sources

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=R589663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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