

Ipsdienone

Inchi: InChI=1S/C10H14O/c1-5-9(4)7-10(11)6-8(2)3/h5-6H,1,4,7H2,2-3H3
InchiKey: RPDIIOSMVGHNKJ-UHFFFAOYSA-N
Formula: C10H14O
SMILES: C=CC(=C)CC(=O)C=C(C)C
Mol. weight [g/mol]: 150.22
CAS: 539-70-8

Physical Properties

Property code	Value	Unit	Source
gf	143.20	kJ/mol	Joback Method
hf	-13.81	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	43.38	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.654		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1152.50		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1152.50		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1145.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1586.00		NIST Webbook
tb	479.35	K	Joback Method
tc	674.39	K	Joback Method
tf	215.87	K	Joback Method
vc	0.545	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.99	J/mol×K	479.35	Joback Method
cpg	303.37	J/mol×K	511.86	Joback Method
cpg	316.00	J/mol×K	544.36	Joback Method
cpg	327.93	J/mol×K	576.87	Joback Method
cpg	339.19	J/mol×K	609.38	Joback Method
cpg	349.82	J/mol×K	641.88	Joback Method
cpg	359.86	J/mol×K	674.39	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=C539708&Units=SI

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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