

Myrcen-8-ol

Inchi:	InChI=1S/C10H16O/c1-4-9(2)6-5-7-10(3)8-11/h4,7,11H,1-2,5-6,8H2,3H3/b10-7+
InchiKey:	IEVYLQISZQFFGA-JXMROGBWSA-N
Formula:	C10H16O
SMILES:	C=CC(=C)CCC=C(C)CO
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	135.30	kJ/mol	Joback Method
hf	-53.46	kJ/mol	Joback Method
hfus	20.77	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.447		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
ripol	1103.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1862.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1862.00		NIST Webbook
tb	517.66	K	Joback Method
tc	693.77	K	Joback Method
tf	226.76	K	Joback Method
vc	0.558	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.15	J/molxK	517.66	Joback Method
cpg	337.23	J/molxK	547.01	Joback Method
cpg	348.70	J/molxK	576.36	Joback Method
cpg	359.60	J/molxK	605.71	Joback Method
cpg	369.96	J/molxK	635.07	Joback Method

cpg	379.80	J/mol×K	664.42	Joback Method
cpg	389.16	J/mol×K	693.77	Joback Method

Sources

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=R227513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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