Myrcenal

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

Physical Properties

Property code	Value	Unit	Source
gf	98.49	kJ/mol	Joback Method
hf	-99.52	kJ/mol	Joback Method
hfus	16.55	kJ/mol	Joback Method
hvap	42.93	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.734		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
ripol	1597.00		NIST Webbook
tb	469.66	K	Joback Method
tc	651.78	K	Joback Method
tf	211.98	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.95	J/mol×K	469.66	Joback Method
cpg	321.51	J/mol×K	500.01	Joback Method
cpg	334.42	J/mol×K	530.37	Joback Method
cpg	346.71	J/mol×K	560.72	Joback Method
cpg	358.40	J/mol×K	591.07	Joback Method
cpg	369.51	J/mol×K	621.43	Joback Method

cpg	380.07	J/mol×K	651.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R193732&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