Novalal

Inchi: InChI=1S/C9H14O/c1-8(2)9(3)6-4-5-7-10/h4-5,7-8H,3,6H2,1-2H3/b5-4-
InchiKey: HVROQZAOTSHMKE-PLNGDYQASA-N
Formula: C9H14O
SMILES: C=C(CC=CC=O)C(C)C
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	82.45	kJ/mol	Joback Method
hf	-87.09	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	41.33	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.344		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	1175.00		NIST Webbook
tb	454.26	K	Joback Method
tc	643.08	K	Joback Method
tf	197.39	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.91	J/mol×K	454.26	Joback Method
cpg	278.76	J/mol×K	485.73	Joback Method
cpg	290.95	J/mol×K	517.20	Joback Method
cpg	302.49	J/mol×K	548.67	Joback Method
cpg	313.42	J/mol×K	580.14	Joback Method
cpg	323.78	J/mol×K	611.61	Joback Method
cpg	333.58	J/mol×K	643.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R503505&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume