Novalic acid

Inchi: InChI=1S/C9H14O2/c1-7(2)8(3)5-4-6-9(10)11/h4,6-7H,3,5H2,1-2H3,(H,10,11)/b6-4-
InchiKey: FYIGSCYMEXOWNZ-XQRVVYSFSA-N
Formula: C9H14O2
SMILES: C=C(CC=CC(=O)O)C(C)C
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-83.77	kJ/mol	Joback Method
hf	-266.32	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	58.03	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.229		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1345.00		NIST Webbook
tb	551.65	K	Joback Method
tc	735.35	K	Joback Method
tf	266.14	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.97	J/mol×K	551.65	Joback Method
cpg	327.96	J/mol×K	582.27	Joback Method
cpg	338.37	J/mol×K	612.88	Joback Method
cpg	348.25	J/mol×K	643.50	Joback Method
cpg	357.60	J/mol×K	674.11	Joback Method
cpg	366.47	J/mol×K	704.73	Joback Method
cpg	374.88	J/mol×K	735.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R503510&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

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