2-ethyl-5-methyl-5-vinyl-tetrahydrofuran

Inchi: InChI=1S/C9H16O/c1-4-8-6-7-9(3,5-2)10-8/h5,8H,2,4,6-7H2,1,3H3
InchiKey: DVPIINWPSFQJCO-UHFFFAOYSA-N
Formula: C9H16O
SMILES: C=CC1(C)CCC(CC)O1
Mol. weight [g/mol]: 140.22
CAS: 104188-14-9

Physical Properties

Property code	Value	Unit	Source
gf	49.97	kJ/mol	Joback Method
hf	-180.28	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	38.27	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.520		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	910.90		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	910.90		NIST Webbook
tb	439.80	K	Joback Method
tc	643.38	K	Joback Method
tf	246.56	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.18	J/mol×K	439.80	Joback Method
cpg	290.35	J/mol×K	473.73	Joback Method
cpg	306.39	J/mol×K	507.66	Joback Method
cpg	321.39	J/mol×K	541.59	Joback Method
cpg	335.46	J/mol×K	575.52	Joback Method

cpg	348.69	J/mol×K	609.45	Joback Method
cpg	361.17	J/mol×K	643.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104188149&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