5-ethylnon-3-en-2-one

Inchi: InChI=1S/C11H20O/c1-4-6-7-11(5-2)9-8-10(3)12/h8-9,11H,4-7H2,1-3H3
InchiKey: SWBGUNASIKSCCO-UHFFFAOYSA-N
Formula: C11H20O
SMILES: CCCCC(C=CC(C)=O)CC
Mol. weight [g/mol]: 168.28
CAS: 10137-90-3

Physical Properties

Property code	Value	Unit	Source
gf	-9.40	kJ/mol	Joback Method
hf	-271.01	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	46.40	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.348		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
tb	508.67	K	Joback Method
tc	691.20	K	Joback Method
tf	243.58	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.23	J/mol×K	508.67	Joback Method
cpg	440.81	J/mol×K	660.78	Joback Method
cpg	428.22	J/mol×K	630.36	Joback Method
cpg	415.00	J/mol×K	599.94	Joback Method
cpg	401.11	J/mol×K	569.51	Joback Method
cpg	386.53	J/mol×K	539.09	Joback Method
cpg	452.78	J/mol×K	691.20	Joback Method
dvisc	0.0001998	Pa×s	508.67	Joback Method
dvisc	0.0002698	Pa×s	464.49	Joback Method

dvisc	0.0003881	Pa×s	420.31	Joback Method
dvisc	0.0006080	Pa×s	376.12	Joback Method
dvisc	0.0010735	Pa×s	331.94	Joback Method
dvisc	0.0022568	Pa×s	287.76	Joback Method
dvisc	0.0062124	Pa×s	243.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10137903&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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume