Tridecanone-

Inchi: InChI=1S/C13H26O/c1-3-4-5-6-7-8-9-10-11-12-13(2)14/h3-12H2,1-2H3
InchiKey: CYIFVRUOHKNECG-UHFFFAOYSA-N
Formula: C13H26O
SMILES: CCCCCCCCCCCC(C)=O
Mol. weight [g/mol]: 198.34
CAS: 57702-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-70.34	kJ/mol	Joback Method
hf	-424.23	kJ/mol	Joback Method
hfus	31.02	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.496		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1505.00		NIST Webbook
tb	550.71	K	Joback Method
tc	719.75	K	Joback Method
tf	286.20	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.12	J/mol×K	550.71	Joback Method
cpg	562.38	J/mol×K	691.58	Joback Method
cpg	548.43	J/mol×K	663.40	Joback Method
cpg	533.84	J/mol×K	635.23	Joback Method
cpg	518.60	J/mol×K	607.06	Joback Method
cpg	502.70	J/mol×K	578.88	Joback Method
cpg	575.73	J/mol×K	719.75	Joback Method

dvisc	0.0002125	Pa×s	550.71	Joback Method
dvisc	0.0002816	Pa×s	506.62	Joback Method
dvisc	0.0003936	Pa×s	462.54	Joback Method
dvisc	0.0005905	Pa×s	418.46	Joback Method
dvisc	0.0009747	Pa×s	374.37	Joback Method
dvisc	0.0018390	Pa×s	330.28	Joback Method
dvisc	0.0042194	Pa×s	286.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57702053&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume