Undecanone

Inchi: InChI=1S/C11H22O/c1-3-4-5-6-7-8-9-10-11(2)12/h3-10H2,1-2H3
InchiKey: KYWIYKKSMDLRDC-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CCCCCCCCCC(C)=O
Mol. weight [g/mol]: 170.29
CAS: 53452-70-3

Physical Properties

Property code	Value	Unit	Source
gf	-87.18	kJ/mol	Joback Method
hf	-382.95	kJ/mol	Joback Method
hfus	25.84	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.716		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1273.00		NIST Webbook
tb	504.95	K	Joback Method
tc	676.40	K	Joback Method
tf	263.66	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.23	J/mol×K	504.95	Joback Method
cpg	403.46	J/mol×K	533.52	Joback Method

cpg	418.07	J/mol×K	562.10	Joback Method
cpg	432.09	J/mol×K	590.67	Joback Method
cpg	445.51	J/mol×K	619.25	Joback Method
cpg	458.36	J/mol×K	647.82	Joback Method
cpg	470.65	J/mol×K	676.40	Joback Method
dvisc	0.0044945	Pa×s	263.66	Joback Method
dvisc	0.0020210	Pa×s	303.88	Joback Method
dvisc	0.0010954	Pa×s	344.09	Joback Method
dvisc	0.0006749	Pa×s	384.30	Joback Method
dvisc	0.0004558	Pa×s	424.52	Joback Method
dvisc	0.0003295	Pa×s	464.74	Joback Method
dvisc	0.0002508	Pa×s	504.95	Joback Method

Sources

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=C53452703&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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