3-Ethyl-3-methyl-2-pentanone

Inchi: InChI=1S/C8H16O/c1-5-8(4,6-2)7(3)9/h5-6H2,1-4H3
InchiKey: VMQCHWRZCMKYGA-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCC(C)(CC)C(C)=O
Mol. weight [g/mol]: 128.21
CAS: 19780-65-5

Physical Properties

Property code	Value	Unit	Source
hf	-330.45	kJ/mol	Cheméo Relay (1.0)
hfus	10.66	kJ/mol	Joback Method
hvap	44.67	kJ/mol	Cheméo Relay (1.0)
ie	8.96	eV	Cheméo Relay (1.0)
log10ws	-1.75		Cheméo Relay (1.0)
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
tb	427.20	K	NIST Webbook
tb	426.00 ± 3.00	K	NIST Webbook
tc	620.62	K	Cheméo Relay (1.0)
tf	253.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.73	J/mol×K	433.08	Joback Method
cpg	271.54	J/mol×K	464.20	Joback Method
cpg	284.66	J/mol×K	495.32	Joback Method
cpg	297.11	J/mol×K	526.44	Joback Method
cpg	308.91	J/mol×K	557.56	Joback Method
cpg	320.09	J/mol×K	588.68	Joback Method
cpg	330.68	J/mol×K	619.80	Joback Method
dvisc	0.0068051	Pa×s	232.27	Joback Method
dvisc	0.0029357	Pa×s	265.74	Joback Method
dvisc	0.0015286	Pa×s	299.21	Joback Method

dvisc	0.0009076	Pa×s	332.67	Joback Method
dvisc	0.0005927	Pa×s	366.14	Joback Method
dvisc	0.0004158	Pa×s	399.61	Joback Method
dvisc	0.0003081	Pa×s	433.08	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49652e+01
Coeff. B	-3.80203e+03
Coeff. C	-5.97450e+01
Temperature range (K), min.	318.78
Temperature range (K), max.	453.58

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19780655&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point