

3-Ethyl-4-octanone

Inchi:	InChI=1S/C10H20O/c1-4-7-8-10(11)9(5-2)6-3/h9H,4-8H2,1-3H3
InchiKey:	XIQNUWMKJWNUCQ-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CCCCC(=O)C(CC)CC
Mol. weight [g/mol]:	156.27
CAS:	19781-29-4

Physical Properties

Property code	Value	Unit	Source
gf	-98.04	kJ/mol	Joback Method
hf	-367.59	kJ/mol	Joback Method
hfus	19.73	kJ/mol	Joback Method
hvap	44.21	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.182		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
tb	481.63	K	Joback Method
tc	658.01	K	Joback Method
tf	237.39	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.14	J/molxK	481.63	Joback Method
cpg	356.94	J/molxK	511.03	Joback Method
cpg	371.13	J/molxK	540.42	Joback Method
cpg	384.72	J/molxK	569.82	Joback Method
cpg	397.72	J/molxK	599.22	Joback Method
cpg	410.16	J/molxK	628.61	Joback Method
cpg	422.05	J/molxK	658.01	Joback Method
dvisc	0.0067728	Paxs	237.39	Joback Method
dvisc	0.0026268	Paxs	278.10	Joback Method

dvisc	0.0012976	Paxs	318.80	Joback Method
dvisc	0.0007520	Paxs	359.51	Joback Method
dvisc	0.0004869	Paxs	400.22	Joback Method
dvisc	0.0003417	Paxs	440.92	Joback Method
dvisc	0.0002545	Paxs	481.63	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=C19781294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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