3-Ethyl-4-heptanone

Other names: 3-Ethyl-4-heptanone
Inchi: InChI=1S/C9H18O/c1-4-7-9(10)8(5-2)6-3/h8H,4-7H2,1-3H3
InchiKey: QMQBUTKELHAKRH-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCC(=O)C(CC)CC
Mol. weight [g/mol]: 142.24

Physical Properties

Property code	Value	Unit	Source
af	0.4464		Cheméo Relay (1.0)
gf	-106.46	kJ/mol	Joback Method
hf	-342.28	kJ/mol	Cheméo Relay (1.0)
hfus	17.14	kJ/mol	Joback Method
hvap	49.85	kJ/mol	Cheméo Relay (1.0)
ie	8.78	eV	Cheméo Relay (1.0)
log10ws	-2.24		Cheméo Relay (1.0)
logp	2.792		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
tb	441.11	K	Cheméo Relay (1.0)
tc	628.53	K	Cheméo Relay (1.0)
tf	223.02	K	Cheméo Relay (1.0)
vc	0.492	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.82	J/mol×K	458.75	Joback Method
cpg	311.71	J/mol×K	488.40	Joback Method
cpg	325.02	J/mol×K	518.05	Joback Method
cpg	337.78	J/mol×K	547.69	Joback Method
cpg	350.00	J/mol×K	577.34	Joback Method
cpg	361.70	J/mol×K	606.99	Joback Method
cpg	372.87	J/mol×K	636.64	Joback Method

dvisc	0.0068479	Pa×s	226.12	Joback Method
dvisc	0.0026929	Pa×s	264.89	Joback Method
dvisc	0.0013439	Pa×s	303.66	Joback Method
dvisc	0.0007850	Pa×s	342.44	Joback Method
dvisc	0.0005116	Pa×s	381.21	Joback Method
dvisc	0.0003608	Pa×s	419.98	Joback Method
dvisc	0.0002699	Pa×s	458.75	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1528252&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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