

Heptanoic acid, 6-oxo-

Other names:	6-oxoheptanoic acid
Inchi:	InChI=1S/C7H12O3/c1-6(8)4-2-3-5-7(9)10/h2-5H2,1H3,(H,9,10)
InchiKey:	IZOQMUVIDMLRDC-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	CC(=O)CCCCC(=O)O
Mol. weight [g/mol]:	144.17
CAS:	3128-07-2

Physical Properties

Property code	Value	Unit	Source
gf	-386.60	kJ/mol	Joback Method
hf	-565.20	kJ/mol	Joback Method
hfus	21.17	kJ/mol	Joback Method
hvap	61.35	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.220		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	559.48	K	Joback Method
tc	738.19	K	Joback Method
tf	329.33	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.04	J/molxK	559.48	Joback Method
cpg	289.21	J/molxK	589.27	Joback Method
cpg	297.96	J/molxK	619.05	Joback Method
cpg	306.30	J/molxK	648.84	Joback Method
cpg	314.24	J/molxK	678.62	Joback Method
cpg	321.79	J/molxK	708.41	Joback Method
cpg	328.96	J/molxK	738.19	Joback Method
dvisc	0.0078882	Paxs	329.33	Joback Method

dvisc	0.0028793	Paxs	367.69	Joback Method
dvisc	0.0012714	Paxs	406.05	Joback Method
dvisc	0.0006465	Paxs	444.40	Joback Method
dvisc	0.0003660	Paxs	482.76	Joback Method
dvisc	0.0002254	Paxs	521.12	Joback Method
dvisc	0.0001483	Paxs	559.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	524.70	K	37.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3128072&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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