6-Oxoheptanoic acid

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

Physical Properties

Property code	Value	Unit	Source
af	0.7454		Cheméo Relay (1.0)
gf	-386.60	kJ/mol	Joback Method
hf	-652.95	kJ/mol	Cheméo Relay (1.0)
hfus	21.17	kJ/mol	Joback Method
hvap	84.27	kJ/mol	Cheméo Relay (1.0)
ie	9.67	eV	Cheméo Relay (1.0)
log10ws	0.03		Cheméo Relay (1.0)
logp	1.220		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	532.78	K	Cheméo Relay (1.0)
tc	711.17	K	Cheméo Relay (1.0)
tf	342.44	K	Cheméo Relay (1.0)
vc	0.432	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0078882	Pa×s	329.33	Joback Method
dvisc	0.0028793	Pa×s	367.69	Joback Method
dvisc	0.0012714	Pa×s	406.05	Joback Method
dvisc	0.0006465	Pa×s	444.41	Joback Method
dvisc	0.0003660	Pa×s	482.76	Joback Method
dvisc	0.0002254	Pa×s	521.12	Joback Method
dvisc	0.0001483	Pa×s	559.48	Joback Method

Pressure Dependent Properties

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3128072&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume