6-methylheptanoic acid

Inchi: InChI=1S/C8H16O2/c1-7(2)5-3-4-6-8(9)10/h7H,3-6H2,1-2H3,(H,9,10)
InchiKey: OEOIWYCWCDBOPA-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CC(C)CCCCC(=O)O
Mol. weight [g/mol]: 144.21
CAS: 25103-52-0

Physical Properties

Property code	Value	Unit	Source
af	0.7215		Cheméo Relay (1.0)
gf	-251.70	kJ/mol	Joback Method
hf	-581.45	kJ/mol	Cheméo Relay (1.0)
hfus	18.64	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Cheméo Relay (1.0)
ie	10.04	eV	Cheméo Relay (1.0)
log10ws	-2.11		Cheméo Relay (1.0)
logp	2.287		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	503.79	K	Cheméo Relay (1.0)
tc	675.91	K	Cheméo Relay (1.0)
tf	286.15	K	Cheméo Relay (1.0)
vc	0.472	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.75	J/mol×K	528.05	Joback Method
cpg	320.87	J/mol×K	556.73	Joback Method
cpg	331.52	J/mol×K	585.41	Joback Method
cpg	341.71	J/mol×K	614.10	Joback Method
cpg	351.46	J/mol×K	642.78	Joback Method
cpg	360.77	J/mol×K	671.46	Joback Method
cpg	369.66	J/mol×K	700.14	Joback Method

dvisc	0.0284980	Pa×s	275.67	Joback Method
dvisc	0.0065326	Pa×s	317.73	Joback Method
dvisc	0.0021132	Pa×s	359.80	Joback Method
dvisc	0.0008658	Pa×s	401.86	Joback Method
dvisc	0.0004201	Pa×s	443.92	Joback Method
dvisc	0.0002310	Pa×s	485.99	Joback Method
dvisc	0.0001397	Pa×s	528.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57061e+01
Coeff. B	-4.67138e+03
Coeff. C	-8.07480e+01
Temperature range (K), min.	383.72
Temperature range (K), max.	530.15

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume