2-ethylpentanoic acid

Inchi: InChI=1S/C7H14O2/c1-3-5-6(4-2)7(8)9/h6H,3-5H2,1-2H3,(H,8,9)
InchiKey: BAZMYXGARXYAEQ-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCCC(CC)C(=O)O
Mol. weight [g/mol]: 130.19
CAS: 20225-24-5

Physical Properties

Property code	Value	Unit	Source
hf	-546.18	kJ/mol	Cheméo Relay (1.0)
hfus	16.05	kJ/mol	Joback Method
hvap	69.69	kJ/mol	Cheméo Relay (1.0)
ie	10.07	eV	Cheméo Relay (1.0)
log10ws	-1.49		Cheméo Relay (1.0)
logp	1.897		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	471.39	K	Cheméo Relay (1.0)
tc	650.26	K	Cheméo Relay (1.0)
tf	229.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.80	J/mol×K	505.17	Joback Method
cpg	276.01	J/mol×K	534.08	Joback Method
cpg	285.78	J/mol×K	562.99	Joback Method
cpg	295.14	J/mol×K	591.90	Joback Method
cpg	304.09	J/mol×K	620.81	Joback Method
cpg	312.64	J/mol×K	649.72	Joback Method
cpg	320.81	J/mol×K	678.63	Joback Method
dvisc	0.0353274	Pa×s	264.40	Joback Method
dvisc	0.0080276	Pa×s	304.53	Joback Method
dvisc	0.0025758	Pa×s	344.66	Joback Method

dvisc	0.0010476	Pa×s	384.78	Joback Method
dvisc	0.0005050	Pa×s	424.91	Joback Method
dvisc	0.0002761	Pa×s	465.04	Joback Method
dvisc	0.0001662	Pa×s	505.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51550e+01
Coeff. B	-4.29902e+03
Coeff. C	-7.52430e+01
Temperature range (K), min.	364.40
Temperature range (K), max.	511.98

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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