2-Ethyl-3-methylhexanoic acid

Inchi: InChI=1S/C9H18O2/c1-4-6-7(3)8(5-2)9(10)11/h7-8H,4-6H2,1-3H3,(H,10,11)
InchiKey: KVHVVWNXJWZHGB-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCC(C)C(CC)C(=O)O
Mol. weight [g/mol]: 158.24
CAS: 74581-94-5

Physical Properties

Property code	Value	Unit	Source
gf	-245.72	kJ/mol	Joback Method
hf	-504.46	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	58.28	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.533		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	550.49	K	Joback Method
tc	724.45	K	Joback Method
tf	271.94	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.90	J/mol×K	550.49	Joback Method
cpg	368.12	J/mol×K	579.48	Joback Method
cpg	379.81	J/mol×K	608.48	Joback Method
cpg	390.98	J/mol×K	637.47	Joback Method
cpg	401.64	J/mol×K	666.46	Joback Method
cpg	411.80	J/mol×K	695.45	Joback Method
cpg	421.50	J/mol×K	724.45	Joback Method
dvisc	0.0424192	Pa×s	271.94	Joback Method
dvisc	0.0076296	Pa×s	318.37	Joback Method

dvisc	0.0021236	Pa×s	364.79	Joback Method
dvisc	0.0007890	Pa×s	411.22	Joback Method
dvisc	0.0003583	Pa×s	457.64	Joback Method
dvisc	0.0001882	Pa×s	504.07	Joback Method
dvisc	0.0001102	Pa×s	550.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44217e+01
Coeff. B	-4.29700e+03
Coeff. C	-8.13040e+01
Temperature range (K), min.	385.32
Temperature range (K), max.	552.97

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C74581945&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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume