3-Ethylheptanoic acid

Inchi: InChI=1S/C9H18O2/c1-3-5-6-8(4-2)7-9(10)11/h8H,3-7H2,1-2H3,(H,10,11)
InchiKey: MCLMZMISZCYBBG-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCCC(CC)CC(=O)O
Mol. weight [g/mol]: 158.24
CAS: 14272-47-0

Physical Properties

Property code	Value	Unit	Source
gf	-243.28	kJ/mol	Joback Method
hf	-499.18	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	58.66	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.678		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
ripol	2048.00		NIST Webbook
tb	509.15 ± 2.00	K	NIST Webbook
tc	721.77	K	Joback Method
tf	286.94	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.57	J/mol×K	550.93	Joback Method
cpg	410.35	J/mol×K	693.29	Joback Method
cpg	400.35	J/mol×K	664.82	Joback Method
cpg	389.89	J/mol×K	636.35	Joback Method
cpg	378.95	J/mol×K	607.88	Joback Method
cpg	367.51	J/mol×K	579.40	Joback Method
cpg	419.88	J/mol×K	721.77	Joback Method
dvisc	0.0001171	Pa×s	550.93	Joback Method

dvisc	0.0001927	Pa×s	506.93	Joback Method
dvisc	0.0003486	Pa×s	462.93	Joback Method
dvisc	0.0007142	Pa×s	418.94	Joback Method
dvisc	0.0017314	Pa×s	374.94	Joback Method
dvisc	0.0053119	Pa×s	330.94	Joback Method
dvisc	0.0229838	Pa×s	286.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54818e+01
Coeff. B	-4.72238e+03
Coeff. C	-8.49180e+01
Temperature range (K), min.	395.72
Temperature range (K), max.	549.25

Sources

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=C14272470&Units=SI

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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume