4-Ethyloctanoic acid

Inchi: InChI=1S/C10H20O2/c1-3-5-6-9(4-2)7-8-10(11)12/h9H,3-8H2,1-2H3,(H,11,12)
InchiKey: PWKJMPFEQOHBAC-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCCCC(CC)CCC(=O)O
Mol. weight [g/mol]: 172.26
CAS: 16493-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-234.86	kJ/mol	Joback Method
hf	-519.82	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	3.068		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1333.00		NIST Webbook
ripol	2216.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2216.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2206.00		NIST Webbook
tb	527.65 ± 4.00	K	NIST Webbook
tc	743.57	K	Joback Method
tf	298.21	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.15	J/mol×K	573.81	Joback Method
cpg	461.31	J/mol×K	715.28	Joback Method
cpg	450.71	J/mol×K	686.99	Joback Method

cpg	439.61	J/mol×K	658.69	Joback Method
cpg	427.99	J/mol×K	630.40	Joback Method
cpg	415.84	J/mol×K	602.10	Joback Method
cpg	471.43	J/mol×K	743.57	Joback Method
dvisc	0.0000979	Pa×s	573.81	Joback Method
dvisc	0.0001605	Pa×s	527.88	Joback Method
dvisc	0.0002888	Pa×s	481.94	Joback Method
dvisc	0.0005884	Pa×s	436.01	Joback Method
dvisc	0.0014176	Pa×s	390.08	Joback Method
dvisc	0.0043186	Pa×s	344.14	Joback Method
dvisc	0.0185428	Pa×s	298.21	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51975e+01
Coeff. B	-4.73522e+03
Coeff. C	-8.85320e+01
Temperature range (K), min.	406.12
Temperature range (K), max.	567.51

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16493804&Units=SI

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

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