5-nonynoic acid

Inchi: InChI=1S/C9H14O2/c1-2-3-4-5-6-7-8-9(10)11/h2-3,6-8H2,1H3,(H,10,11)
InchiKey: GIMQQWKASGCRDK-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CCCC#CCCCC(=O)O
Mol. weight [g/mol]: 154.21
CAS: 56630-34-3

Physical Properties

Property code	Value	Unit	Source
af	0.6697		Cheméo Relay (1.0)
gf	-38.04	kJ/mol	Joback Method
hf	-309.06	kJ/mol	Cheméo Relay (1.0)
hfus	27.88	kJ/mol	Joback Method
hvap	86.60	kJ/mol	Cheméo Relay (1.0)
ie	9.60	eV	Cheméo Relay (1.0)
log10ws	-1.57		Cheméo Relay (1.0)
logp	2.045		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	517.79	K	Cheméo Relay (1.0)
tc	718.06	K	Cheméo Relay (1.0)
tf	298.20	K	Cheméo Relay (1.0)
vc	0.483	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.89	J/mol×K	560.37	Joback Method
cpg	328.66	J/mol×K	591.44	Joback Method
cpg	338.94	J/mol×K	622.52	Joback Method
cpg	348.75	J/mol×K	653.59	Joback Method
cpg	358.10	J/mol×K	684.67	Joback Method
cpg	367.00	J/mol×K	715.74	Joback Method
cpg	375.48	J/mol×K	746.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57239e+01
Coeff. B	-5.31769e+03
Coeff. C	-1.02860e+02
Temperature range (K), min.	447.15
Temperature range (K), max.	613.15

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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