2-propylheptanoic acid

Inchi: InChI=1S/C10H20O2/c1-3-5-6-8-9(7-4-2)10(11)12/h9H,3-8H2,1-2H3,(H,11,12)
InchiKey: RXGPYPPCEXISOV-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCCCCC(CCC)C(=O)O
Mol. weight [g/mol]: 172.27
CAS: 31080-39-4

Physical Properties

Property code	Value	Unit	Source
af	0.7503		Cheméo Relay (1.0)
gf	-234.86	kJ/mol	Joback Method
hf	-603.13	kJ/mol	Cheméo Relay (1.0)
hfus	23.82	kJ/mol	Joback Method
hvap	77.00	kJ/mol	Cheméo Relay (1.0)
ie	9.91	eV	Cheméo Relay (1.0)
log10ws	-3.10		Cheméo Relay (1.0)
logp	3.068		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	515.65	K	Cheméo Relay (1.0)
tc	701.93	K	Cheméo Relay (1.0)
tf	251.84	K	Cheméo Relay (1.0)
vc	0.575	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.15	J/mol×K	573.81	Joback Method
cpg	471.43	J/mol×K	743.57	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

dvisc	0.0005884	Pa×s	436.01	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	0.0185428	Pa×s	298.21	Joback Method
dvisc	0.0014176	Pa×s	390.08	Joback Method
dvisc	0.0043186	Pa×s	344.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55358e+01
Coeff. B	-4.87449e+03
Coeff. C	-8.96440e+01
Temperature range (K), min.	409.32
Temperature range (K), max.	566.40

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

af:	Acentric Factor
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
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