Tricosanoic acid

Other names: n-Tricosanoic acid
Inchi: InChI=1S/C23H46O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24
InchiKey: XEZVDURJDFGERA-UHFFFAOYSA-N
Formula: C23H46O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 354.61
CAS: 2433-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-122.96	kJ/mol	Joback Method
hf	-782.86	kJ/mol	Joback Method
hfus	61.01	kJ/mol	Joback Method
hvap	90.22	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	8.283		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	934.63	kPa	Joback Method
rinpol	2668.10		NIST Webbook
tb	871.69	K	Joback Method
tc	1069.35	K	Joback Method
tf	324.40 ± 3.00	K	NIST Webbook
tf	339.00 ± 4.00	K	NIST Webbook
tf	351.90 ± 2.00	K	NIST Webbook
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1246.66	J/mol×K	1069.35	Joback Method
cpg	1231.46	J/mol×K	1036.41	Joback Method
cpg	1215.36	J/mol×K	1003.46	Joback Method
cpg	1198.29	J/mol×K	970.52	Joback Method
cpg	1180.19	J/mol×K	937.58	Joback Method

cpg	1161.00	J/mol×K	904.63	Joback Method
cpg	1140.68	J/mol×K	871.69	Joback Method
dvisc	0.0009361	Pa×s	459.72	Joback Method
dvisc	0.0000097	Pa×s	871.69	Joback Method
dvisc	0.0000150	Pa×s	803.03	Joback Method
dvisc	0.0000252	Pa×s	734.37	Joback Method
dvisc	0.0000471	Pa×s	665.70	Joback Method
dvisc	0.0001014	Pa×s	597.04	Joback Method
dvisc	0.0002667	Pa×s	528.38	Joback Method
hfust	75.00	kJ/mol	352.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.04425e+01
Coeff. B	-8.65242e+03
Coeff. C	-1.48024e+02
Temperature range (K), min.	577.32
Temperature range (K), max.	719.86

Sources

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=C2433967&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

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume