14-methylpentadecanoic acid

Inchi: InChI=1S/C16H32O2/c1-15(2)13-11-9-7-5-3-4-6-8-10-12-14-16(17)18/h15H,3-14H2,1-2H
InchiKey: ZONJATNKKGGVSU-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CC(C)CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 256.42
CAS: 4669-02-7

Physical Properties

Property code	Value	Unit	Source
gf	-184.34	kJ/mol	Joback Method
hf	-643.66	kJ/mol	Joback Method
hfus	39.36	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.408		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
ripol	2861.00		NIST Webbook
ripol	2861.00		NIST Webbook
tb	711.09	K	Joback Method
tc	881.15	K	Joback Method
tf	335.00 ± 1.50	K	NIST Webbook
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.27	J/mol×K	711.09	Joback Method
cpg	736.41	J/mol×K	739.43	Joback Method
cpg	751.80	J/mol×K	767.78	Joback Method
cpg	766.47	J/mol×K	796.12	Joback Method
cpg	780.45	J/mol×K	824.46	Joback Method
cpg	793.76	J/mol×K	852.80	Joback Method
cpg	806.41	J/mol×K	881.15	Joback Method

dvisc	0.0052083	Pa×s	365.83	Joback Method
dvisc	0.0012596	Pa×s	423.37	Joback Method
dvisc	0.0004279	Pa×s	480.92	Joback Method
dvisc	0.0001831	Pa×s	538.46	Joback Method
dvisc	0.0000923	Pa×s	596.00	Joback Method
dvisc	0.0000525	Pa×s	653.55	Joback Method
dvisc	0.0000327	Pa×s	711.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62950e+01
Coeff. B	-5.88592e+03
Coeff. C	-1.15220e+02
Temperature range (K), min.	482.92
Temperature range (K), max.	651.11

Sources

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=C4669027&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

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