Tridecanoic acid, 12-methyl

Other names: 12-METHYL TRICADENOIC ACID
12-methyltridecanoic acid
Inchi: InChI=1S/C14H28O2/c1-13(2)11-9-7-5-3-4-6-8-10-12-14(15)16/h13H,3-12H2,1-2H3,(H,1
InchiKey: YYVJAABUJYRQJO-UHFFFAOYSA-N
Formula: C14H28O2
SMILES: CC(C)CCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 228.37
CAS: 2724-57-4

Physical Properties

Property code	Value	Unit	Source
gf	-201.18	kJ/mol	Joback Method
hf	-602.38	kJ/mol	Joback Method
hfus	34.18	kJ/mol	Joback Method
hvap	69.80	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.628		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
ripol	2657.00		NIST Webbook
ripol	2657.00		NIST Webbook
tb	665.33	K	Joback Method
tc	833.65	K	Joback Method
tf	328.00 ± 2.00	K	NIST Webbook
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.14	J/mol×K	665.33	Joback Method
cpg	678.14	J/mol×K	805.60	Joback Method
cpg	665.61	J/mol×K	777.54	Joback Method
cpg	652.47	J/mol×K	749.49	Joback Method
cpg	638.69	J/mol×K	721.44	Joback Method

cpg	624.25	J/mol×K	693.38	Joback Method
cpg	690.08	J/mol×K	833.65	Joback Method
dvisc	0.0000473	Pa×s	665.33	Joback Method
dvisc	0.0000763	Pa×s	611.66	Joback Method
dvisc	0.0001351	Pa×s	557.98	Joback Method
dvisc	0.0002702	Pa×s	504.31	Joback Method
dvisc	0.0006370	Pa×s	450.64	Joback Method
dvisc	0.0018944	Pa×s	396.96	Joback Method
dvisc	0.0079212	Pa×s	343.29	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58185e+01
Coeff. B	-5.45940e+03
Coeff. C	-1.06602e+02
Temperature range (K), min.	458.12
Temperature range (K), max.	626.20

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=C2724574&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