Tridecanedioic acid

Other names:	.alpha.,.omega.-tridecanedioic acid
	1,11-Undecanedicarboxylic acid
	1,13-Tridecanedioic acid
	Brassilic acid
	Brassylic acid
Inchi:	InChI=1S/C13H24O4/c14-12(15)10-8-6-4-2-1-3-5-7-9-11-13(16)17/h1-11H2,(H,14,15)(H,
InchiKey:	DXNCZXXFRKPEPY-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	O=C(O)CCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	244.33
CAS:	505-52-2

Physical Properties

Property code	Value	Unit	Source
chs	-7397.30 ± 3.30	kJ/mol	NIST Webbook
gf	-472.90	kJ/mol	Joback Method
hf	-841.27	kJ/mol	Joback Method
hfus	49.40	kJ/mol	Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16
hvap	91.38	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.447		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
tb	788.94	K	Joback Method
tc	968.90	K	Joback Method
tf	387.50 ± 0.50	K	NIST Webbook
tf	386.21	K	Solubility of tridecanedioic acid in pure solvent systems: An experimental and computational study
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.23	J/mol×K	908.91	Joback Method
cpg	696.66	J/mol×K	968.90	Joback Method
cpg	687.71	J/mol×K	938.90	Joback Method
cpg	634.46	J/mol×K	788.94	Joback Method
cpg	646.32	J/mol×K	818.93	Joback Method
cpg	657.56	J/mol×K	848.93	Joback Method
cpg	668.18	J/mol×K	878.92	Joback Method
dvisc	0.0000077	Pa×s	788.94	Joback Method
dvisc	0.0000237	Pa×s	678.55	Joback Method
dvisc	0.0000129	Pa×s	733.74	Joback Method
dvisc	0.0011525	Pa×s	457.77	Joback Method
dvisc	0.0003189	Pa×s	512.96	Joback Method
dvisc	0.0001133	Pa×s	568.16	Joback Method
dvisc	0.0000483	Pa×s	623.36	Joback Method
hfust	49.40	kJ/mol	386.30	NIST Webbook
hfust	45.30	kJ/mol	387.50	NIST Webbook
sfust	116.90	J/mol×K	387.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53406e+01
Coeff. B	-6.02945e+03
Coeff. C	-1.26323e+02
Temperature range (K), min.	526.87
Temperature range (K), max.	727.52

Sources

Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16:	https://www.doi.org/10.1016/j.jct.2004.12.011
Solubility of tridecanedioic acid in pure solvent systems: An experimental and computational study:	https://www.doi.org/10.1016/j.jct.2015.05.026

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=C505522&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

chs:	Standard solid enthalpy of combustion
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume