13-(cyclopent-2-enyl)tridecanoic acid

Other names: 13-(2-cyclopenten-1-yl)tridecanoic acid
Inchi: InChI=1S/C18H32O2/c19-18(20)16-10-8-6-4-2-1-3-5-7-9-13-17-14-11-12-15-17/h11,14,1
InchiKey: XMVQWNRDPAAMJB-KRWDZBQOSA-N
Formula: C18H32O2
SMILES: O=C(O)CCCCCCCCCCCCC1C=CCC1
Mol. weight [g/mol]: 280.45
CAS: 29106-32-9

Physical Properties

Property code	Value	Unit	Source
gf	-98.55	kJ/mol	Joback Method
hf	-561.40	kJ/mol	Joback Method
hfus	43.22	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.718		Crippen Method
mcvol	256.760	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2230.50		NIST Webbook
rinpol	2230.50		NIST Webbook
tb	771.73	K	Joback Method
tc	955.37	K	Joback Method
tf	341.30 ± 2.00	K	NIST Webbook
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.58	J/mol×K	771.73	Joback Method
cpg	818.49	J/mol×K	802.34	Joback Method
cpg	834.49	J/mol×K	832.94	Joback Method
cpg	849.63	J/mol×K	863.55	Joback Method
cpg	863.94	J/mol×K	894.16	Joback Method
cpg	877.46	J/mol×K	924.76	Joback Method

cpg	890.25	J/mol×K	955.37	Joback Method
dvisc	0.0025117	Pa×s	415.03	Joback Method
dvisc	0.0008009	Pa×s	474.48	Joback Method
dvisc	0.0003294	Pa×s	533.93	Joback Method
dvisc	0.0001619	Pa×s	593.38	Joback Method
dvisc	0.0000905	Pa×s	652.83	Joback Method
dvisc	0.0000558	Pa×s	712.28	Joback Method
dvisc	0.0000370	Pa×s	771.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29106329&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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