isopentadecanoic acid

Inchi: InChI=1S/C15H30O2/c1-14(2)12-10-8-6-4-3-5-7-9-11-13-15(16)17/h14H,3-13H2,1-2H3,(
InchiKey: ZOCYQVNGROEVLU-UHFFFAOYSA-N
Formula: C15H30O2
SMILES: CC(C)CCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 242.40
CAS: 50973-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-192.76	kJ/mol	Joback Method
hf	-623.02	kJ/mol	Joback Method
hfus	36.77	kJ/mol	Joback Method
hvap	72.02	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	5.018		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1856.00		NIST Webbook
tb	688.21	K	Joback Method
tc	857.15	K	Joback Method
tf	354.56	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.10	J/mol×K	688.21	Joback Method
cpg	679.73	J/mol×K	716.37	Joback Method
cpg	694.65	J/mol×K	744.52	Joback Method
cpg	708.88	J/mol×K	772.68	Joback Method
cpg	722.45	J/mol×K	800.84	Joback Method
cpg	735.38	J/mol×K	828.99	Joback Method
cpg	747.69	J/mol×K	857.15	Joback Method

dvisc	0.0064199	Pa×s	354.56	Joback Method
dvisc	0.0015442	Pa×s	410.17	Joback Method
dvisc	0.0005220	Pa×s	465.78	Joback Method
dvisc	0.0002224	Pa×s	521.38	Joback Method
dvisc	0.0001117	Pa×s	576.99	Joback Method
dvisc	0.0000633	Pa×s	632.60	Joback Method
dvisc	0.0000393	Pa×s	688.21	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50973096&Units=SI

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