

PENTADECANEDIOIC ACID

Other names:	Pentadecanedioic acid
Inchi:	InChI=1S/C15H28O4/c16-14(17)12-10-8-6-4-2-1-3-5-7-9-11-13-15(18)19/h1-13H2,(H,16
InchiKey:	BTZVDPWKGXMQFW-UHFFFAOYSA-N
Formula:	C15H28O4
SMILES:	O=C(O)CCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
af	1.1772		Cheméo Relay (1.0)
gf	-456.06	kJ/mol	Joback Method
hf	-1022.64	kJ/mol	Cheméo Relay (1.0)
hfus	45.98	kJ/mol	Joback Method
hvap	145.79	kJ/mol	Cheméo Relay (1.0)
ie	9.79	eV	Cheméo Relay (1.0)
log10ws	-4.24		Cheméo Relay (1.0)
logp	4.227		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
tb	593.32	K	Cheméo Relay (1.0)
tc	818.00	K	Cheméo Relay (1.0)
tf	399.07	K	Cheméo Relay (1.0)
vc	0.908	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.12	J/mol×K	834.70	Joback Method
cpg	815.41	J/mol×K	1022.11	Joback Method
cpg	805.66	J/mol×K	990.87	Joback Method
cpg	795.30	J/mol×K	959.64	Joback Method
cpg	784.30	J/mol×K	928.40	Joback Method
cpg	772.62	J/mol×K	897.17	Joback Method
cpg	760.24	J/mol×K	865.93	Joback Method

dvisc	0.0000306	Pa×s	657.50	Joback Method
dvisc	0.0000049	Pa×s	834.70	Joback Method
dvisc	0.0000082	Pa×s	775.63	Joback Method
dvisc	0.0000150	Pa×s	716.57	Joback Method
dvisc	0.0007293	Pa×s	480.31	Joback Method
dvisc	0.0000714	Pa×s	598.44	Joback Method
dvisc	0.0002009	Pa×s	539.38	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1460180&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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