Hexadecanoic acid, 9,10,16-trihydroxy-, (R*,S*)-(.+/-.)-

Other names: «alpha»-Aleuritic acid
9,10,16-Trihydroxypalmitic acid
DL-erythro-9,10,16-Trihydroxyhexadecanoic acid
Hexadecanoic acid, 9,10,16-trihydroxy-, erythro-, dl-
8,9,15-Trihydroxypentadecane-1-carboxylic acid
9,10,16-Trihydroxyhexadecanoic acid
(.+/-.)-erythro-Aleuritic acid
DL-erythro-Aleuritic acid
erythro-Aleuritic acid
NSC 7668
Aleuritic acid

Inchi: InChI=1S/C16H32O5/c17-13-9-5-4-7-11-15(19)14(18)10-6-2-1-3-8-12-16(20)21/h14-15,1

InchiKey: MEHUJCGAYMDLEL-UHFFFAOYSA-N

Formula: C16H32O5

SMILES: O=C(O)CCCCCCCC(O)C(O)CCCCCCO

Mol. weight [g/mol]: 304.42

CAS: 533-87-9

Physical Properties

Property code	Value	Unit	Source
gf	-597.24	kJ/mol	Joback Method
hf	-1105.63	kJ/mol	Joback Method
hfus	48.10	kJ/mol	Joback Method
hvap	123.90	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.466		Crippen Method
mcvol	261.350	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
tb	987.19	K	Joback Method
tc	1234.29	K	Joback Method
tf	533.29	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.94	J/mol×K	987.19	Joback Method
cpg	919.43	J/mol×K	1028.37	Joback Method
cpg	932.86	J/mol×K	1069.56	Joback Method
cpg	945.31	J/mol×K	1110.74	Joback Method
cpg	956.88	J/mol×K	1151.93	Joback Method
cpg	967.64	J/mol×K	1193.11	Joback Method
cpg	977.70	J/mol×K	1234.29	Joback Method
dvisc	0.0000856	Pa×s	533.29	Joback Method
dvisc	0.0000105	Pa×s	608.94	Joback Method
dvisc	0.0000020	Pa×s	684.59	Joback Method
dvisc	0.0000005	Pa×s	760.24	Joback Method
dvisc	0.0000002	Pa×s	835.89	Joback Method
dvisc	7.6780938e-08	Pa×s	911.54	Joback Method
dvisc	3.5977590e-08	Pa×s	987.19	Joback Method

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=C533879&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume