

cis-10-Heptadecenoic acid

Inchi:	InChI=1S/C17H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19/h7-8H,2-6,9-16
InchiKey:	GDTXICBNEOEPAZ-FPLPWBNLSA-N
Formula:	C17H32O2
SMILES:	CCCCCCC=CCCCCCCCC(=O)O
Mol. weight [g/mol]:	268.43
CAS:	29743-97-3

Physical Properties

Property code	Value	Unit	Source
gf	-93.26	kJ/mol	Joback Method
hf	-541.80	kJ/mol	Joback Method
hfus	45.68	kJ/mol	Joback Method
hvap	76.82	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.718		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	2073.20		NIST Webbook
tb	738.57	K	Joback Method
tc	912.25	K	Joback Method
tf	387.02	K	Joback Method
vc	0.993	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.53	J/mol×K	738.57	Joback Method
cpg	826.18	J/mol×K	883.30	Joback Method
cpg	813.00	J/mol×K	854.36	Joback Method
cpg	799.18	J/mol×K	825.41	Joback Method
cpg	784.69	J/mol×K	796.46	Joback Method
cpg	769.49	J/mol×K	767.52	Joback Method
cpg	838.74	J/mol×K	912.25	Joback Method
dvisc	0.0000252	Paxs	738.57	Joback Method

dvisc	0.0000395	Paxs	679.98	Joback Method
dvisc	0.0000674	Paxs	621.39	Joback Method
dvisc	0.0001285	Paxs	562.79	Joback Method
dvisc	0.0002846	Paxs	504.20	Joback Method
dvisc	0.0007775	Paxs	445.61	Joback Method
dvisc	0.0028789	Paxs	387.02	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=C29743973&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
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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