

12-Chloropentadecanoic acid, methyl ester

Inchi:	InChI=1S/C16H31ClO2/c1-3-12-15(17)13-10-8-6-4-5-7-9-11-14-16(18)19-2/h15H,3-14H2
InchiKey:	GMNWRBPDFDZYHH-UHFFFAOYSA-N
Formula:	C16H31ClO2
SMILES:	CCCC(Cl)CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	290.87

Physical Properties

Property code	Value	Unit	Source
gf	-164.45	kJ/mol	Joback Method
hf	-639.39	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.468		Crippen Method
mcvol	255.980	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2013.00		NIST Webbook
ripol	2484.00		NIST Webbook
ripol	2484.00		NIST Webbook
tb	678.76	K	Joback Method
tc	853.20	K	Joback Method
tf	357.16	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.02	J/molxK	678.76	Joback Method
cpg	789.95	J/molxK	824.12	Joback Method
cpg	775.70	J/molxK	795.05	Joback Method
cpg	760.71	J/molxK	765.98	Joback Method
cpg	744.94	J/molxK	736.91	Joback Method
cpg	728.39	J/molxK	707.83	Joback Method

cpg	803.46	J/mol×K	853.20	Joback Method
dvisc	0.0001020	Paxs	678.76	Joback Method
dvisc	0.0001380	Paxs	625.16	Joback Method
dvisc	0.0001977	Paxs	571.56	Joback Method
dvisc	0.0003050	Paxs	517.96	Joback Method
dvisc	0.0005200	Paxs	464.36	Joback Method
dvisc	0.0010191	Paxs	410.76	Joback Method
dvisc	0.0024442	Paxs	357.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308904&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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