

12-Chlorododecanoic acid, methyl ester

Inchi:	InChI=1S/C13H25ClO2/c1-16-13(15)11-9-7-5-3-2-4-6-8-10-12-14/h2-12H2,1H3
InchiKey:	ULWCBDZJKRGIOK-UHFFFAOYSA-N
Formula:	C13H25ClO2
SMILES:	COC(=O)CCCCCCCCCCCCI
Mol. weight [g/mol]:	248.79

Physical Properties

Property code	Value	Unit	Source
gf	-187.27	kJ/mol	Joback Method
hf	-572.19	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.299		Crippen Method
mcvol	213.710	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1769.00		NIST Webbook
rinpol	1769.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2234.00		NIST Webbook
tb	610.56	K	Joback Method
tc	784.07	K	Joback Method
tf	338.35	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.83	J/molxK	610.56	Joback Method
cpg	563.46	J/molxK	639.48	Joback Method
cpg	578.43	J/molxK	668.40	Joback Method
cpg	592.72	J/molxK	697.32	Joback Method
cpg	606.37	J/molxK	726.24	Joback Method
cpg	619.38	J/molxK	755.15	Joback Method

cpg	631.77	J/molxK	784.07	Joback Method
dvisc	0.0024461	Paxs	338.35	Joback Method
dvisc	0.0011849	Paxs	383.72	Joback Method
dvisc	0.0006691	Paxs	429.09	Joback Method
dvisc	0.0004215	Paxs	474.45	Joback Method
dvisc	0.0002878	Paxs	519.82	Joback Method
dvisc	0.0002089	Paxs	565.19	Joback Method
dvisc	0.0001590	Paxs	610.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308860&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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