

6-Chlorododecanoic acid, methyl ester

Inchi:	InChI=1S/C13H25ClO2/c1-3-4-5-6-9-12(14)10-7-8-11-13(15)16-2/h12H,3-11H2,1-2H3
InchiKey:	CCSZZBKTQWDMMT-UHFFFAOYSA-N
Formula:	C13H25ClO2
SMILES:	CCCCCCC(Cl)CCCC(=O)OC
Mol. weight [g/mol]:	248.79

Physical Properties

Property code	Value	Unit	Source
gf	-189.71	kJ/mol	Joback Method
hf	-577.47	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.298		Crippen Method
mcvol	213.710	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpola	1691.00		NIST Webbook
ripola	2113.00		NIST Webbook
tb	610.12	K	Joback Method
tc	786.44	K	Joback Method
tf	323.35	K	Joback Method
vc	0.831	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.21	J/molxK	610.12	Joback Method
cpg	620.96	J/molxK	757.05	Joback Method
cpg	607.77	J/molxK	727.67	Joback Method
cpg	593.91	J/molxK	698.28	Joback Method
cpg	579.37	J/molxK	668.89	Joback Method
cpg	564.14	J/molxK	639.51	Joback Method
cpg	633.51	J/molxK	786.44	Joback Method
dvisc	0.0001484	Paxs	610.12	Joback Method

dvisc	0.0001991	Paxs	562.33	Joback Method
dvisc	0.0002822	Paxs	514.53	Joback Method
dvisc	0.0004297	Paxs	466.74	Joback Method
dvisc	0.0007200	Paxs	418.94	Joback Method
dvisc	0.0013781	Paxs	371.14	Joback Method
dvisc	0.0031957	Paxs	323.35	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=R309610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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