5-Chlorododecanoic acid, methyl ester

Inchi: InChI=1S/C13H25ClO2/c1-3-4-5-6-7-9-12(14)10-8-11-13(15)16-2/h12H,3-11H2,1-2H3
InchiKey: YBJNBGQMYONEGO-UHFFFAOYSA-N
Formula: C13H25ClO2
SMILES: CCCCCCCC(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
rinpol	1683.00		NIST Webbook
rinpol	1683.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
tb	610.12	K	Joback Method
tc	786.44	K	Joback Method
tf	323.35	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.21	J/mol×K	610.12	Joback Method
cpg	564.14	J/mol×K	639.51	Joback Method
cpg	579.37	J/mol×K	668.89	Joback Method
cpg	593.91	J/mol×K	698.28	Joback Method
cpg	607.77	J/mol×K	727.67	Joback Method
cpg	620.96	J/mol×K	757.05	Joback Method

cpg	633.51	J/mol×K	786.44	Joback Method
dvisc	0.0031957	Pa×s	323.35	Joback Method
dvisc	0.0013781	Pa×s	371.14	Joback Method
dvisc	0.0007200	Pa×s	418.94	Joback Method
dvisc	0.0004297	Pa×s	466.74	Joback Method
dvisc	0.0002822	Pa×s	514.53	Joback Method
dvisc	0.0001991	Pa×s	562.33	Joback Method
dvisc	0.0001484	Pa×s	610.12	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=R309487&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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