Lauric acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C18H26Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-18(21)22-15-12-13-16(19)17(20)14-15
InchiKey: WCWAWFAFRNCXRQ-UHFFFAOYSA-N
Formula: C18H26Cl2O2
SMILES: CCCCCCCCCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 345.30

Physical Properties

Property code	Value	Unit	Source
gf	-63.95	kJ/mol	Joback Method
hf	-477.54	kJ/mol	Joback Method
hfus	46.82	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.820		Crippen Method
mcvol	272.640	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
rinpol	2477.00		NIST Webbook
rinpol	2477.00		NIST Webbook
tb	799.03	K	Joback Method
tc	1000.94	K	Joback Method
tf	476.08	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.37	J/mol×K	799.03	Joback Method
cpg	784.77	J/mol×K	832.68	Joback Method
cpg	799.19	J/mol×K	866.33	Joback Method
cpg	812.66	J/mol×K	899.98	Joback Method
cpg	825.22	J/mol×K	933.63	Joback Method
cpg	836.89	J/mol×K	967.28	Joback Method
cpg	847.71	J/mol×K	1000.94	Joback Method
dvisc	0.0007171	Pa×s	476.08	Joback Method

dvisc	0.0004077	Pa×s	529.90	Joback Method
dvisc	0.0002572	Pa×s	583.73	Joback Method
dvisc	0.0001754	Pa×s	637.55	Joback Method
dvisc	0.0001269	Pa×s	691.38	Joback Method
dvisc	0.0000963	Pa×s	745.20	Joback Method
dvisc	0.0000758	Pa×s	799.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357927&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

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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