Nonanoic acid, 3,4-dichlorophenyl ester

Other names: Nonoic acid, 3,4-dichlorophenyl ester
Inchi: InChI=1S/C15H20Cl2O2/c1-2-3-4-5-6-7-8-15(18)19-12-9-10-13(16)14(17)11-12/h9-11H,2
InchiKey: GLRDUADSTVKNMV-UHFFFAOYSA-N
Formula: C15H20Cl2O2
SMILES: CCCCCCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 303.22

Physical Properties

Property code	Value	Unit	Source
gf	-89.21	kJ/mol	Joback Method
hf	-415.62	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.649		Crippen Method
mcvol	230.370	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2147.00		NIST Webbook
tb	730.39	K	Joback Method
tc	936.84	K	Joback Method
tf	442.27	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.51	J/mol×K	730.39	Joback Method
cpg	616.91	J/mol×K	764.80	Joback Method
cpg	630.42	J/mol×K	799.21	Joback Method
cpg	643.05	J/mol×K	833.61	Joback Method
cpg	654.84	J/mol×K	868.02	Joback Method
cpg	665.81	J/mol×K	902.43	Joback Method
cpg	675.98	J/mol×K	936.84	Joback Method
dvisc	0.0009239	Pa×s	442.27	Joback Method

dvisc	0.0005473	Pa×s	490.29	Joback Method
dvisc	0.0003559	Pa×s	538.31	Joback Method
dvisc	0.0002484	Pa×s	586.33	Joback Method
dvisc	0.0001830	Pa×s	634.35	Joback Method
dvisc	0.0001408	Pa×s	682.37	Joback Method
dvisc	0.0001121	Pa×s	730.39	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U358027&Units=SI

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