Nonanoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C15H19Cl3O2/c1-2-3-4-5-6-7-8-15(19)20-14-10-12(17)11(16)9-13(14)18/h9-10
InchiKey: CRUCWHJNZNUXBY-UHFFFAOYSA-N
Formula: C15H19Cl3O2
SMILES: CCCCCCCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 337.67

Physical Properties

Property code	Value	Unit	Source
gf	-110.77	kJ/mol	Joback Method
hf	-442.83	kJ/mol	Joback Method
hfus	42.86	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	6.303		Crippen Method
mcvol	242.610	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	772.80	K	Joback Method
tc	983.51	K	Joback Method
tf	484.71	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.11	J/mol×K	772.80	Joback Method
cpg	684.82	J/mol×K	948.39	Joback Method
cpg	674.95	J/mol×K	913.27	Joback Method
cpg	664.27	J/mol×K	878.15	Joback Method
cpg	652.75	J/mol×K	843.04	Joback Method
cpg	640.37	J/mol×K	807.92	Joback Method
cpg	693.89	J/mol×K	983.51	Joback Method
dvisc	0.0001000	Pa×s	772.80	Joback Method

dvisc	0.0001237	Pa×s	724.78	Joback Method
dvisc	0.0001578	Pa×s	676.77	Joback Method
dvisc	0.0002088	Pa×s	628.75	Joback Method
dvisc	0.0002895	Pa×s	580.74	Joback Method
dvisc	0.0004257	Pa×s	532.73	Joback Method
dvisc	0.0006757	Pa×s	484.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360673&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume