

Octanoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C14H18Cl2O2/c1-2-3-4-5-6-7-14(17)18-11-8-9-12(15)13(16)10-11/h8-10H,2-7H
InchiKey: XRHJWXJKQKYIBL-UHFFFAOYSA-N
Formula: C14H18Cl2O2
SMILES: CCCCCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 289.20

Physical Properties

Property code	Value	Unit	Source
gf	-97.63	kJ/mol	Joback Method
hf	-394.98	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	68.28	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.259		Crippen Method
mcvol	216.280	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1998.00		NIST Webbook
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tb	707.51	K	Joback Method
tc	916.48	K	Joback Method
tf	431.00	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.14	J/molxK	707.51	Joback Method
cpg	563.11	J/molxK	742.34	Joback Method
cpg	576.22	J/molxK	777.17	Joback Method
cpg	588.48	J/molxK	811.99	Joback Method
cpg	599.92	J/molxK	846.82	Joback Method
cpg	610.57	J/molxK	881.65	Joback Method
cpg	620.43	J/molxK	916.48	Joback Method
dvisc	0.0009939	Paxs	431.00	Joback Method

dvisc	0.0005975	Paxs	477.08	Joback Method
dvisc	0.0003929	Paxs	523.17	Joback Method
dvisc	0.0002765	Paxs	569.25	Joback Method
dvisc	0.0002051	Paxs	615.34	Joback Method
dvisc	0.0001586	Paxs	661.42	Joback Method
dvisc	0.0001268	Paxs	707.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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