Propanoic acid, 2,3-dichloro, isohexyl ester

Other names: Propanoic acid, 2,3-dichloro, 4-methylpentyl ester
Inchi: InChI=1S/C9H16Cl2O2/c1-7(2)4-3-5-13-9(12)8(11)6-10/h7-8H,3-6H2,1-2H3
InchiKey: GLLAESMJKBMUAC-UHFFFAOYSA-N
Formula: C9H16Cl2O2
SMILES: CC(C)CCCOC(=O)C(Cl)CCl
Mol. weight [g/mol]: 227.13

Physical Properties

Property code	Value	Unit	Source
gf	-237.76	kJ/mol	Joback Method
hf	-515.93	kJ/mol	Joback Method
hfus	23.20	kJ/mol	Joback Method
hvap	52.78	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.812		Crippen Method
mcvol	169.590	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1243.00		NIST Webbook
ripol	1714.00		NIST Webbook
tb	555.59	K	Joback Method
tc	746.91	K	Joback Method
tf	293.19	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.69	J/mol×K	555.59	Joback Method
cpg	438.99	J/mol×K	715.02	Joback Method
cpg	428.50	J/mol×K	683.14	Joback Method
cpg	417.43	J/mol×K	651.25	Joback Method
cpg	405.78	J/mol×K	619.36	Joback Method
cpg	393.54	J/mol×K	587.48	Joback Method
cpg	448.92	J/mol×K	746.91	Joback Method

dvisc	0.0002033	Pa×s	555.59	Joback Method
dvisc	0.0002742	Pa×s	511.86	Joback Method
dvisc	0.0003910	Pa×s	468.12	Joback Method
dvisc	0.0005999	Pa×s	424.39	Joback Method
dvisc	0.0010155	Pa×s	380.66	Joback Method
dvisc	0.0019708	Pa×s	336.92	Joback Method
dvisc	0.0046613	Pa×s	293.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30232&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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