

Isobutyric acid, alpha-chloro-2,4-dichloro phenyl ester

Inchi:	InChI=1S/C10H9Cl3O2/c1-10(2,13)9(14)15-6-3-4-7(11)8(12)5-6/h3-5H,1-2H3
InchiKey:	COOMWMJTGCTXAY-UHFFFAOYSA-N
Formula:	C10H9Cl3O2
SMILES:	CC(C)(Cl)C(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	267.54

Physical Properties

Property code	Value	Unit	Source
gf	-140.40	kJ/mol	Joback Method
hf	-336.91	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.916		Crippen Method
mcvol	172.160	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	650.19	K	Joback Method
tc	890.08	K	Joback Method
tf	418.26	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.31	J/molxK	650.19	Joback Method
cpg	386.22	J/molxK	690.17	Joback Method
cpg	396.26	J/molxK	730.15	Joback Method
cpg	405.45	J/molxK	770.13	Joback Method
cpg	413.86	J/molxK	810.11	Joback Method
cpg	421.53	J/molxK	850.10	Joback Method
cpg	428.50	J/molxK	890.08	Joback Method
dvisc	0.0011373	Paxs	418.26	Joback Method
dvisc	0.0007134	Paxs	456.92	Joback Method
dvisc	0.0004813	Paxs	495.57	Joback Method

dvisc	0.0003437	Paxs	534.23	Joback Method
dvisc	0.0002569	Paxs	572.88	Joback Method
dvisc	0.0001992	Paxs	611.54	Joback Method
dvisc	0.0001592	Paxs	650.19	Joback Method

Sources

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=B6001978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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