

Methyl 2,2-dichloropentanoate

Inchi:	InChI=1S/C6H10Cl2O2/c1-3-4-6(7,8)5(9)10-2/h3-4H2,1-2H3
InchiKey:	IZTMVFSJBDVCCA-UHFFFAOYSA-N
Formula:	C6H10Cl2O2
SMILES:	CCCC(Cl)(Cl)C(=O)OC
Mol. weight [g/mol]:	185.05

Physical Properties

Property code	Value	Unit	Source
gf	-255.30	kJ/mol	Joback Method
hf	-452.20	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	45.58	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.133		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
tb	484.60	K	Joback Method
tc	687.13	K	Joback Method
tf	291.80	K	Joback Method
vc	0.482	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.33	J/mol×K	484.60	Joback Method
cpg	262.47	J/mol×K	518.36	Joback Method
cpg	272.04	J/mol×K	552.11	Joback Method
cpg	281.06	J/mol×K	585.87	Joback Method
cpg	289.55	J/mol×K	619.62	Joback Method
cpg	297.52	J/mol×K	653.38	Joback Method
cpg	305.00	J/mol×K	687.13	Joback Method
dvisc	0.0036475	Paxs	291.80	Joback Method

dvisc	0.0019601	Paxs	323.93	Joback Method
dvisc	0.0011783	Paxs	356.07	Joback Method
dvisc	0.0007706	Paxs	388.20	Joback Method
dvisc	0.0005377	Paxs	420.33	Joback Method
dvisc	0.0003949	Paxs	452.47	Joback Method
dvisc	0.0003022	Paxs	484.60	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=R80344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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