

Dimethyl 2,2-dichlorobutanedioate

Inchi:	InChI=1S/C6H8Cl2O4/c1-11-4(9)3-6(7,8)5(10)12-2/h3H2,1-2H3
InchiKey:	UKJLCUUEQJDIOP-UHFFFAOYSA-N
Formula:	C6H8Cl2O4
SMILES:	COC(=O)CC(Cl)(Cl)C(=O)OC
Mol. weight [g/mol]:	215.03

Physical Properties

Property code	Value	Unit	Source
gf	-489.22	kJ/mol	Joback Method
hf	-697.00	kJ/mol	Joback Method
hfus	17.85	kJ/mol	Joback Method
hvap	54.74	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.896		Crippen Method
mcvol	134.760	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1182.00		NIST Webbook
tb	560.89	K	Joback Method
tc	770.51	K	Joback Method
tf	363.96	K	Joback Method
vc	0.506	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.69	J/mol×K	560.89	Joback Method
cpg	294.68	J/mol×K	595.83	Joback Method
cpg	303.15	J/mol×K	630.76	Joback Method
cpg	311.10	J/mol×K	665.70	Joback Method
cpg	318.53	J/mol×K	700.64	Joback Method
cpg	325.45	J/mol×K	735.58	Joback Method
cpg	331.87	J/mol×K	770.51	Joback Method
dvisc	0.0019696	Paxs	363.96	Joback Method
dvisc	0.0011959	Paxs	396.78	Joback Method

dvisc	0.0007837	Paxs	429.60	Joback Method
dvisc	0.0005453	Paxs	462.43	Joback Method
dvisc	0.0003981	Paxs	495.25	Joback Method
dvisc	0.0003022	Paxs	528.07	Joback Method
dvisc	0.0002370	Paxs	560.89	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=R80219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
mccvol:	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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