METHYL 2,4-DICHLOROBUTANOATE

Other names: 2,4-Dichlorobutanoic acid, methyl ester
Inchi: InChI=1S/C5H8Cl2O2/c1-9-5(8)4(7)2-3-6/h4H,2-3H2,1H3
InchiKey: MIXXUSQBRXDJHD-UHFFFAOYSA-N
Formula: C5H8Cl2O2
SMILES: COC(=O)C(Cl)CCCl
Mol. weight [g/mol]: 171.02

Physical Properties

Property code	Value	Unit	Source
af	0.4228		Cheméo Relay (1.0)
hf	-496.32	kJ/mol	Cheméo Relay (1.0)
hfus	16.36	kJ/mol	Joback Method
hvap	55.74	kJ/mol	Cheméo Relay (1.0)
ie	10.56	eV	Cheméo Relay (1.0)
log10ws	-1.46		Cheméo Relay (1.0)
logp	1.396		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1057.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1056.00		NIST Webbook
tb	451.28	K	Cheméo Relay (1.0)
tc	660.46	K	Cheméo Relay (1.0)
tf	239.32	K	Cheméo Relay (1.0)
vc	0.395	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.55	J/mol×K	464.51	Joback Method
cpg	217.82	J/mol×K	497.33	Joback Method
cpg	225.76	J/mol×K	530.15	Joback Method
cpg	233.34	J/mol×K	562.97	Joback Method
cpg	240.59	J/mol×K	595.78	Joback Method

cpg	247.49	J/mol×K	628.60	Joback Method
cpg	254.06	J/mol×K	661.42	Joback Method
dvisc	0.0039296	Pa×s	263.11	Joback Method
dvisc	0.0020352	Pa×s	296.68	Joback Method
dvisc	0.0012050	Pa×s	330.24	Joback Method
dvisc	0.0007858	Pa×s	363.81	Joback Method
dvisc	0.0005509	Pa×s	397.38	Joback Method
dvisc	0.0004081	Pa×s	430.94	Joback Method
dvisc	0.0003158	Pa×s	464.51	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62093656&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume