Malonic acid, butyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C9H14Cl2O4/c1-2-3-4-14-8(12)5-9(13)15-6-7(10)11/h7H,2-6H2,1H3
InchiKey: OXMJTLDSJUOPRS-UHFFFAOYSA-N
Formula: C9H14Cl2O4
SMILES: CCCCOC(=O)CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 257.11

Physical Properties

Property code	Value	Unit	Source
gf	-469.24	kJ/mol	Joback Method
hf	-755.45	kJ/mol	Joback Method
hfus	29.51	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.067		Crippen Method
mcvol	177.030	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1557.00		NIST Webbook
tb	632.32	K	Joback Method
tc	826.21	K	Joback Method
tf	380.35	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.84	J/mol×K	632.32	Joback Method
cpg	472.05	J/mol×K	793.90	Joback Method
cpg	462.98	J/mol×K	761.58	Joback Method
cpg	453.33	J/mol×K	729.27	Joback Method
cpg	443.08	J/mol×K	696.95	Joback Method
cpg	432.25	J/mol×K	664.64	Joback Method
cpg	480.52	J/mol×K	826.21	Joback Method
dvisc	0.0001696	Pa×s	632.32	Joback Method
dvisc	0.0002191	Pa×s	590.32	Joback Method

dvisc	0.0002944	Pa×s	548.33	Joback Method
dvisc	0.0004153	Pa×s	506.33	Joback Method
dvisc	0.0006234	Pa×s	464.34	Joback Method
dvisc	0.0010147	Pa×s	422.34	Joback Method
dvisc	0.0018392	Pa×s	380.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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