Dimethyl 2,3-Dibromo-1,4-butanedioate, (2R,3R)-rel-

Other names: Butanedicarbonic acid,-2,3-dibromo, dimethyl ester
Butanedioic acid, 2,3-dibromo-, 1,4-dimethyl ester, (2R,3R)-rel-
Inchi: InChI=1S/C6H8Br2O4/c1-11-5(9)3(7)4(8)6(10)12-2/h3-4H,1-2H3
InchiKey: XQBOXCHKENCESQ-UHFFFAOYSA-N
Formula: C6H8Br2O4
SMILES: COC(=O)C(Br)C(Br)C(=O)OC
Mol. weight [g/mol]: 303.93
CAS: 1186-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-444.44	kJ/mol	Joback Method
hf	-614.67	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	59.36	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.859		Crippen Method
mcvol	145.280	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	620.70	K	Joback Method
tc	844.02	K	Joback Method
tf	391.30	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.69	J/mol×K	620.70	Joback Method
cpg	308.37	J/mol×K	657.92	Joback Method
cpg	316.52	J/mol×K	695.14	Joback Method
cpg	324.14	J/mol×K	732.36	Joback Method
cpg	331.21	J/mol×K	769.58	Joback Method
cpg	337.76	J/mol×K	806.80	Joback Method
cpg	343.77	J/mol×K	844.02	Joback Method

dvisc	0.0017841	Pa×s	391.30	Joback Method
dvisc	0.0010677	Pa×s	429.53	Joback Method
dvisc	0.0006949	Pa×s	467.77	Joback Method
dvisc	0.0004826	Pa×s	506.00	Joback Method
dvisc	0.0003527	Pa×s	544.23	Joback Method
dvisc	0.0002687	Pa×s	582.47	Joback Method
dvisc	0.0002116	Pa×s	620.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1186987&Units=SI

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