

Dimethyl 1-bromoethylmalonate

Inchi:	InChI=1S/C7H11BrO4/c1-4(8)5(6(9)11-2)7(10)12-3/h4-5H,1-3H3
InchiKey:	FPEOKHVGTMWSAN-UHFFFAOYSA-N
Formula:	C7H11BrO4
SMILES:	COC(=O)C(C(=O)OC)C(C)Br
Mol. weight [g/mol]:	239.06

Physical Properties

Property code	Value	Unit	Source
gf	-450.34	kJ/mol	Joback Method
hf	-661.64	kJ/mol	Joback Method
hfus	17.70	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.732		Crippen Method
mcvol	141.870	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1340.00		NIST Webbook
tb	577.42	K	Joback Method
tc	784.68	K	Joback Method
tf	342.77	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.02	J/molxK	577.42	Joback Method
cpg	324.52	J/molxK	611.96	Joback Method
cpg	334.51	J/molxK	646.51	Joback Method
cpg	343.97	J/molxK	681.05	Joback Method
cpg	352.90	J/molxK	715.59	Joback Method
cpg	361.30	J/molxK	750.14	Joback Method
cpg	369.16	J/molxK	784.68	Joback Method
dvisc	0.0025054	Paxs	342.77	Joback Method
dvisc	0.0013512	Paxs	381.88	Joback Method

dvisc	0.0008173	Paxs	420.99	Joback Method
dvisc	0.0005385	Paxs	460.09	Joback Method
dvisc	0.0003788	Paxs	499.20	Joback Method
dvisc	0.0002804	Paxs	538.31	Joback Method
dvisc	0.0002162	Paxs	577.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R80205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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