

Ethyl dibromoacetate

Other names:	Acetic acid, dibromo-, ethyl ester Dibromoacetic acid, ethyl ester
Inchi:	InChI=1S/C4H6Br2O2/c1-2-8-4(7)3(5)6/h3H,2H2,1H3
InchiKey:	NIJGVVHCUXNSLL-UHFFFAOYSA-N
Formula:	C4H6Br2O2
SMILES:	CCOC(=O)C(Br)Br
Mol. weight [g/mol]:	245.90
CAS:	617-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-224.92	kJ/mol	Joback Method
hf	-323.31	kJ/mol	Joback Method
hfus	15.95	kJ/mol	Joback Method
hvap	46.14	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.665		Crippen Method
mvol	109.660	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	467.20	K	NIST Webbook
tc	720.07	K	Joback Method
tf	311.60	K	Joback Method
vc	0.402	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.60	J/molxK	499.09	Joback Method
cpg	217.73	J/molxK	683.24	Joback Method
cpg	212.25	J/molxK	646.41	Joback Method
cpg	206.40	J/molxK	609.58	Joback Method
cpg	200.19	J/molxK	572.75	Joback Method
cpg	193.59	J/molxK	535.92	Joback Method
cpg	222.87	J/molxK	720.07	Joback Method

dvisc	0.0003676	Paxs	499.09	Joback Method
dvisc	0.0004592	Paxs	467.84	Joback Method
dvisc	0.0005922	Paxs	436.59	Joback Method
dvisc	0.0007943	Paxs	405.35	Joback Method
dvisc	0.0011189	Paxs	374.10	Joback Method
dvisc	0.0016778	Paxs	342.85	Joback Method
dvisc	0.0027287	Paxs	311.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.20	K	9.90	NIST Webbook

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=C617334&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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

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