

Acetic acid, dibromo-, methyl ester

Other names:	Methyl dibromoacetate
Inchi:	InChI=1S/C3H4Br2O2/c1-7-3(6)2(4)5/h2H,1H3
InchiKey:	DZFMUIJZSYIMPH-UHFFFAOYSA-N
Formula:	C3H4Br2O2
SMILES:	COC(=O)C(Br)Br
Mol. weight [g/mol]:	231.87
CAS:	6482-26-4

Physical Properties

Property code	Value	Unit	Source
gf	-233.34	kJ/mol	Joback Method
hf	-302.67	kJ/mol	Joback Method
hfus	13.36	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.275		Crippen Method
mcvol	95.570	ml/mol	McGowan Method
pc	5791.74	kPa	Joback Method
rinpol	966.00		NIST Webbook
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tb	476.21	K	Joback Method
tc	700.86	K	Joback Method
tf	300.33	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.77	J/molxK	476.21	Joback Method
cpg	173.18	J/molxK	663.42	Joback Method
cpg	168.89	J/molxK	625.98	Joback Method
cpg	164.31	J/molxK	588.54	Joback Method
cpg	159.44	J/molxK	551.09	Joback Method
cpg	154.27	J/molxK	513.65	Joback Method

cpg	177.19	J/mol×K	700.86	Joback Method
dvisc	0.0004073	Paxs	476.21	Joback Method
dvisc	0.0005055	Paxs	446.90	Joback Method
dvisc	0.0006468	Paxs	417.58	Joback Method
dvisc	0.0008589	Paxs	388.27	Joback Method
dvisc	0.0011945	Paxs	358.96	Joback Method
dvisc	0.0017618	Paxs	329.64	Joback Method
dvisc	0.0028033	Paxs	300.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6482264&Units=SI
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

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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