

Acetic acid, dibromo, 1-methylpropyl ester

Inchi:	InChI=1S/C6H10Br2O2/c1-3-4(2)10-6(9)5(7)8/h4-5H,3H2,1-2H3
InchiKey:	PNWWZNZTEYSBAW-UHFFFAOYSA-N
Formula:	C6H10Br2O2
SMILES:	CCC(C)OC(=O)C(Br)Br
Mol. weight [g/mol]:	273.95

Physical Properties

Property code	Value	Unit	Source
gf	-210.52	kJ/mol	Joback Method
hf	-369.87	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.444		Crippen Method
mcvol	137.840	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	1169.00		NIST Webbook
rinpol	1169.00		NIST Webbook
ripol	1663.00		NIST Webbook
tb	544.41	K	Joback Method
tc	762.87	K	Joback Method
tf	319.14	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.87	J/molxK	544.41	Joback Method
cpg	278.66	J/molxK	580.82	Joback Method
cpg	287.88	J/molxK	617.23	Joback Method
cpg	296.57	J/molxK	653.64	Joback Method
cpg	304.73	J/molxK	690.05	Joback Method
cpg	312.38	J/molxK	726.46	Joback Method
cpg	319.55	J/molxK	762.87	Joback Method

dvisc	0.0031975	Paxs	319.14	Joback Method
dvisc	0.0017149	Paxs	356.69	Joback Method
dvisc	0.0010356	Paxs	394.23	Joback Method
dvisc	0.0006828	Paxs	431.77	Joback Method
dvisc	0.0004812	Paxs	469.32	Joback Method
dvisc	0.0003571	Paxs	506.86	Joback Method
dvisc	0.0002762	Paxs	544.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115683&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

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

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