

Acetic acid, dibromo, 3-methylbutyl ester

Inchi:	InChI=1S/C7H12Br2O2/c1-5(2)3-4-11-7(10)6(8)9/h5-6H,3-4H2,1-2H3
InchiKey:	YFVZXEFPWZTPNG-UHFFFAOYSA-N
Formula:	C7H12Br2O2
SMILES:	CC(C)CCOC(=O)C(Br)Br
Mol. weight [g/mol]:	287.98

Physical Properties

Property code	Value	Unit	Source
gf	-202.10	kJ/mol	Joback Method
hf	-390.51	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	52.43	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.692		Crippen Method
mcvol	151.930	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
ripol	1296.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1807.00		NIST Webbook
tb	567.29	K	Joback Method
tc	782.01	K	Joback Method
tf	330.41	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.74	J/molxK	567.29	Joback Method
cpg	323.57	J/molxK	603.08	Joback Method
cpg	333.79	J/molxK	638.86	Joback Method
cpg	343.42	J/molxK	674.65	Joback Method
cpg	352.47	J/molxK	710.44	Joback Method
cpg	360.97	J/molxK	746.23	Joback Method
cpg	368.94	J/molxK	782.01	Joback Method

dvisc	0.0029934	Paxs	330.41	Joback Method
dvisc	0.0015774	Paxs	369.89	Joback Method
dvisc	0.0009406	Paxs	409.37	Joback Method
dvisc	0.0006143	Paxs	448.85	Joback Method
dvisc	0.0004298	Paxs	488.33	Joback Method
dvisc	0.0003172	Paxs	527.81	Joback Method
dvisc	0.0002442	Paxs	567.29	Joback Method

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=R115707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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