Acetic acid, dibromo, 1-methylethyl ester

Inchi: InChI=1S/C5H8Br2O2/c1-3(2)9-5(8)4(6)7/h3-4H,1-2H3
InchiKey: VIGRSXFVWKMQLH-UHFFFAOYSA-N
Formula: C5H8Br2O2
SMILES: CC(C)OC(=O)C(Br)Br
Mol. weight [g/mol]: 259.92

Physical Properties

Property code	Value	Unit	Source
gf	-218.94	kJ/mol	Joback Method
hf	-349.23	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	47.97	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.054		Crippen Method
mcvol	123.750	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
rinpol	1068.00		NIST Webbook
rinpol	1068.00		NIST Webbook
ripol	1574.00		NIST Webbook
tb	521.53	K	Joback Method
tc	743.83	K	Joback Method
tf	307.87	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.90	J/mol×K	521.53	Joback Method
cpg	235.49	J/mol×K	558.58	Joback Method
cpg	243.59	J/mol×K	595.63	Joback Method
cpg	251.20	J/mol×K	632.68	Joback Method
cpg	258.35	J/mol×K	669.73	Joback Method
cpg	265.05	J/mol×K	706.78	Joback Method
cpg	271.31	J/mol×K	743.83	Joback Method

dvisc	0.0033859	Pa×s	307.87	Joback Method
dvisc	0.0018501	Pa×s	343.48	Joback Method
dvisc	0.0011325	Pa×s	379.09	Joback Method
dvisc	0.0007542	Pa×s	414.70	Joback Method
dvisc	0.0005356	Pa×s	450.31	Joback Method
dvisc	0.0004000	Pa×s	485.92	Joback Method
dvisc	0.0003108	Pa×s	521.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115678&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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