

Acetic acid, tribromo, 1,1-dimethylethyl ester

Inchi:	InChI=1S/C6H9Br3O2/c1-5(2,3)11-4(10)6(7,8)9/h1-3H3
InchiKey:	NNWAVDRLTUJGLU-UHFFFAOYSA-N
Formula:	C6H9Br3O2
SMILES:	CC(C)(C)OC(=O)C(Br)(Br)Br
Mol. weight [g/mol]:	352.85

Physical Properties

Property code	Value	Unit	Source
gf	-185.64	kJ/mol	Joback Method
hf	-350.48	kJ/mol	Joback Method
hfus	15.11	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.167		Crippen Method
mcvol	155.340	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook
tb	604.99	K	Joback Method
tc	856.30	K	Joback Method
tf	413.78	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.72	J/molxK	604.99	Joback Method
cpg	343.56	J/molxK	814.42	Joback Method
cpg	337.39	J/molxK	772.53	Joback Method
cpg	330.63	J/molxK	730.65	Joback Method
cpg	323.17	J/molxK	688.76	Joback Method
cpg	314.90	J/molxK	646.88	Joback Method
cpg	349.25	J/molxK	856.30	Joback Method
dvisc	0.0002105	Paxs	604.99	Joback Method

dvisc	0.0002668	Paxs	573.12	Joback Method
dvisc	0.0003478	Paxs	541.25	Joback Method
dvisc	0.0004686	Paxs	509.38	Joback Method
dvisc	0.0006570	Paxs	477.52	Joback Method
dvisc	0.0009667	Paxs	445.65	Joback Method
dvisc	0.0015096	Paxs	413.78	Joback Method

Sources

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=R115772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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