

4-Penten-2-ol, tribromoacetate

Inchi:	InChI=1S/C7H9Br3O2/c1-3-4-5(2)12-6(11)7(8,9)10/h3,5H,1,4H2,2H3
InchiKey:	HHZMCGURKPTEQC-UHFFFAOYSA-N
Formula:	C7H9Br3O2
SMILES:	C=CCC(C)OC(=O)C(Br)(Br)Br
Mol. weight [g/mol]:	364.86

Physical Properties

Property code	Value	Unit	Source
gf	-94.66	kJ/mol	Joback Method
hf	-242.22	kJ/mol	Joback Method
hfus	20.31	kJ/mol	Joback Method
hvap	57.28	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.333		Crippen Method
mcvol	165.130	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinqol	1436.00		NIST Webbook
tb	627.34	K	Joback Method
tc	868.59	K	Joback Method
tf	405.87	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.72	J/molxK	627.34	Joback Method
cpg	335.84	J/molxK	667.55	Joback Method
cpg	344.18	J/molxK	707.76	Joback Method
cpg	351.82	J/molxK	747.97	Joback Method
cpg	358.85	J/molxK	788.17	Joback Method
cpg	365.32	J/molxK	828.38	Joback Method
cpg	371.34	J/molxK	868.59	Joback Method
dvisc	0.0016108	Paxs	405.87	Joback Method
dvisc	0.0009828	Paxs	442.78	Joback Method

dvisc	0.0006471	Paxs	479.69	Joback Method
dvisc	0.0004522	Paxs	516.61	Joback Method
dvisc	0.0003315	Paxs	553.52	Joback Method
dvisc	0.0002526	Paxs	590.43	Joback Method
dvisc	0.0001988	Paxs	627.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R26578&Units=SI

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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