

4-Penten-1-ol, tribromoacetate

Inchi:	InChI=1S/C7H9Br3O2/c1-2-3-4-5-12-6(11)7(8,9)10/h2H,1,3-5H2
InchiKey:	VYTCVMXDJCMLLL-UHFFFAOYSA-N
Formula:	C7H9Br3O2
SMILES:	C=CCCCOC(=O)C(Br)(Br)Br
Mol. weight [g/mol]:	364.86

Physical Properties

Property code	Value	Unit	Source
gf	-92.22	kJ/mol	Joback Method
hf	-236.94	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.334		Crippen Method
mcvol	165.130	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinsol	1513.00		NIST Webbook
tb	627.78	K	Joback Method
tc	863.89	K	Joback Method
tf	420.87	K	Joback Method
vc	0.608	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.18	J/molxK	627.78	Joback Method
cpg	335.06	J/molxK	667.13	Joback Method
cpg	343.20	J/molxK	706.48	Joback Method
cpg	350.69	J/molxK	745.84	Joback Method
cpg	357.59	J/molxK	785.19	Joback Method
cpg	363.98	J/molxK	824.54	Joback Method
cpg	369.93	J/molxK	863.89	Joback Method
dvisc	0.0013630	Paxs	420.87	Joback Method
dvisc	0.0008902	Paxs	455.36	Joback Method

dvisc	0.0006173	Paxs	489.84	Joback Method
dvisc	0.0004492	Paxs	524.33	Joback Method
dvisc	0.0003400	Paxs	558.81	Joback Method
dvisc	0.0002657	Paxs	593.29	Joback Method
dvisc	0.0002134	Paxs	627.78	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=R26500&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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