

Trifluoroacetic acid, cyclopentyl ester

Other names:	Acetic acid, trifluoro-, cyclopentyl ester
Inchi:	InChI=1S/C7H9F3O2/c8-7(9,10)6(11)12-5-3-1-2-4-5/h5H,1-4H2
InchiKey:	QCONYJQZFUESJD-UHFFFAOYSA-N
Formula:	C7H9F3O2
SMILES:	O=C(OC1CCCC1)C(F)(F)F
Mol. weight [g/mol]:	182.14
CAS:	703-13-9

Physical Properties

Property code	Value	Unit	Source
gf	-770.90	kJ/mol	Joback Method
hf	-969.21	kJ/mol	Joback Method
hfus	12.43	kJ/mol	Joback Method
hvap	36.84	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.034		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	445.71	K	Joback Method
tc	632.89	K	Joback Method
tf	255.90	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.41	J/molxK	445.71	Joback Method
cpg	261.71	J/molxK	476.91	Joback Method
cpg	274.28	J/molxK	508.10	Joback Method
cpg	286.13	J/molxK	539.30	Joback Method
cpg	297.28	J/molxK	570.50	Joback Method
cpg	307.78	J/molxK	601.69	Joback Method
cpg	317.63	J/molxK	632.89	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=C703139&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
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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