

Trifluoroacetic acid, 2-methylpropyl ester

Other names:	Isobutyl trifluoroacetate Isobutyl trifluoroacetate Acetic acid, trifluoro-, 2-methylpropyl ester Trifluoroacetic acid, isobutyl ester
Inchi:	InChI=1S/C6H9F3O2/c1-4(2)3-11-5(10)6(7,8)9/h4H,3H2,1-2H3
InchiKey:	JNDIDDMPBOLGER-UHFFFAOYSA-N
Formula:	C6H9F3O2
SMILES:	CC(C)COC(=O)C(F)(F)F
Mol. weight [g/mol]:	170.13
CAS:	17355-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-818.31	kJ/mol	Joback Method
hf	-1014.33	kJ/mol	Joback Method
hfus	12.39	kJ/mol	Joback Method
hvap	33.97	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.748		Crippen Method
mcvol	108.150	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	653.00		NIST Webbook
rinpol	625.40		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	656.40		NIST Webbook
rinpol	625.40		NIST Webbook
tb	407.11	K	Joback Method
tc	572.02	K	Joback Method
tf	218.73	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	226.82	J/mol×K	407.11	Joback Method
cpg	236.72	J/mol×K	434.60	Joback Method
cpg	246.20	J/mol×K	462.08	Joback Method
cpg	255.25	J/mol×K	489.57	Joback Method
cpg	263.89	J/mol×K	517.05	Joback Method
cpg	272.12	J/mol×K	544.54	Joback Method
cpg	279.97	J/mol×K	572.02	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=C17355838&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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