Acetic acid, trifluoro-, 3-methylbutyl ester

Other names:	Trifluoroacetic acid, 3-methylbutyl ester
	3-Methyl-1-butanol, trifluoroacetate
	Isopentyl trifluoroacetate
Inchi:	InChI=1S/C7H11F3O2/c1-5(2)3-4-12-6(11)7(8,9)10/h5H,3-4H2,1-2H3
InchiKey:	UOUKEYVAKRKVQA-UHFFFAOYSA-N
Formula:	C7H11F3O2
SMILES:	CC(C)CCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	184.16
CAS:	327-69-5

Physical Properties

Property code	Value	Unit	Source
gf	-809.89	kJ/mol	Joback Method
hf	-1034.97	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	36.20	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.138		Crippen Method
mcvol	122.240	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	759.20		NIST Webbook
rinpol	724.90		NIST Webbook
rinpol	752.10		NIST Webbook
tb	429.99	K	Joback Method
tc	594.24	K	Joback Method
tf	230.00	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.92	J/mol×K	429.99	Joback Method
cpg	276.90	J/mol×K	457.36	Joback Method
cpg	287.40	J/mol×K	484.74	Joback Method

cpg	297.44	J/mol×K	512.11	Joback Method
cpg	307.02	J/mol×K	539.49	Joback Method
cpg	316.16	J/mol×K	566.86	Joback Method
cpg	324.86	J/mol×K	594.24	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=C327695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/40-993-5/Acetic-acid-trifluoro-3-methylbutyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:19:35.166564531 +0000 UTC m=+3284037.803533780.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.