

Trifluoroacetic acid, heptyl ester

Other names:	Heptyl trifluoroacetate Acetic acid, trifluoro, heptyl ester
Inchi:	InChI=1S/C9H15F3O2/c1-2-3-4-5-6-7-14-8(13)9(10,11)12/h2-7H2,1H3
InchiKey:	UYLWXQBGISCNKI-UHFFFAOYSA-N
Formula:	C9H15F3O2
SMILES:	CCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	212.21
CAS:	2710-89-6

Physical Properties

Property code	Value	Unit	Source
gf	-790.61	kJ/mol	Joback Method
hf	-1070.97	kJ/mol	Joback Method
hfus	23.68	kJ/mol	Joback Method
hvap	41.04	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.062		Crippen Method
mcvol	150.420	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	968.00		NIST Webbook
rinpol	927.20		NIST Webbook
rinpol	927.20		NIST Webbook
rinpol	971.80		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	940.00		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1073.00		NIST Webbook
ripol	1070.00		NIST Webbook
tb	438.65 ± 1.50	K	NIST Webbook
tc	635.68	K	Joback Method
tf	267.54	K	Joback Method
vc	0.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.37	J/molxK	476.19	Joback Method
cpg	362.87	J/molxK	502.77	Joback Method
cpg	374.85	J/molxK	529.35	Joback Method
cpg	386.30	J/molxK	555.94	Joback Method
cpg	397.25	J/molxK	582.52	Joback Method
cpg	407.71	J/molxK	609.10	Joback Method
cpg	417.70	J/molxK	635.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2710896&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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