

Acetic acid, trifluoro, N,N-dipropyl

Inchi:	InChI=1S/C8H14F3NO/c1-3-5-12(6-4-2)7(13)8(9,10)11/h3-6H2,1-2H3
InchiKey:	LSZMQYWSYFXIKW-UHFFFAOYSA-N
Formula:	C8H14F3NO
SMILES:	CCCN(CCC)C(=O)C(F)(F)F
Mol. weight [g/mol]:	197.20

Physical Properties

Property code	Value	Unit	Source
gf	-583.25	kJ/mol	Joback Method
hf	-850.58	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	38.44	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.197		Crippen Method
mcvol	140.440	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinsol	1040.00		NIST Webbook
tb	443.33	K	Joback Method
tc	602.13	K	Joback Method
tf	266.51	K	Joback Method
vc	0.550	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.47	J/mol×K	443.33	Joback Method
cpg	326.27	J/mol×K	469.80	Joback Method
cpg	338.44	J/mol×K	496.26	Joback Method
cpg	350.02	J/mol×K	522.73	Joback Method
cpg	361.02	J/mol×K	549.20	Joback Method
cpg	371.47	J/mol×K	575.67	Joback Method
cpg	381.39	J/mol×K	602.13	Joback Method

Sources

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=R120155&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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