

Acetamide, N-tetrahydrofurfuryl-2,2,2-trifluoro-

Inchi:	InChI=1S/C7H10F3NO2/c8-7(9,10)6(12)11-4-5-2-1-3-13-5/h5H,1-4H2,(H,11,12)
InchiKey:	QRYQSMKXOLWVRX-UHFFFAOYSA-N
Formula:	C7H10F3NO2
SMILES:	O=C(NCC1CCCO1)C(F)(F)F
Mol. weight [g/mol]:	197.16

Physical Properties

Property code	Value	Unit	Source
gf	-662.63	kJ/mol	Joback Method
hf	-915.52	kJ/mol	Joback Method
hfus	24.32	kJ/mol	Joback Method
hvap	45.38	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	0.844		Crippen Method
mcvol	121.360	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	673.00		NIST Webbook
tb	500.41	K	Joback Method
tc	690.86	K	Joback Method
tf	312.90	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.72	J/mol×K	500.41	Joback Method
cpg	313.94	J/mol×K	532.15	Joback Method
cpg	326.32	J/mol×K	563.89	Joback Method
cpg	337.91	J/mol×K	595.63	Joback Method
cpg	348.75	J/mol×K	627.38	Joback Method
cpg	358.86	J/mol×K	659.12	Joback Method
cpg	368.28	J/mol×K	690.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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