Acetamide, N-butyl-2,2,2-trifluoro-

Other names: N-Butyltrifluoroacetamide
CF3C(O)NH(CH2)3CH3
CF3CONH(n-C4H9)
Inchi: InChI=1S/C6H10F3NO/c1-2-3-4-10-5(11)6(7,8)9/h2-4H2,1H3,(H,10,11)
InchiKey: BIBAVAVHXLGIBU-UHFFFAOYSA-N
Formula: C6H10F3NO
SMILES: CCCCNC(=O)C(F)(F)F
Mol. weight [g/mol]: 169.14
CAS: 400-59-9

Physical Properties

Property code	Value	Unit	Source
affp	850.30	kJ/mol	NIST Webbook
basg	819.40	kJ/mol	NIST Webbook
gf	-621.48	kJ/mol	Joback Method
hf	-823.36	kJ/mol	Joback Method
hfus	19.82	kJ/mol	Joback Method
hvap	38.38	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.465		Crippen Method
mcvol	112.260	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	435.30	K	Joback Method
tc	601.02	K	Joback Method
tf	264.16	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.84	J/mol×K	435.30	Joback Method
cpg	256.25	J/mol×K	462.92	Joback Method
cpg	266.14	J/mol×K	490.54	Joback Method
cpg	275.53	J/mol×K	518.16	Joback Method

cpg	284.42	J/mol×K	545.78	Joback Method
cpg	292.84	J/mol×K	573.40	Joback Method
cpg	300.82	J/mol×K	601.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C400599&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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