Benzamide, 2,3,4-trifluoro-N-methyl-

Inchi: InChI=1S/C8H6F3NO/c1-12-8(13)4-2-3-5(9)7(11)6(4)10/h2-3H,1H3,(H,12,13)
InchiKey: YKIMXPNCTGWWHV-UHFFFAOYSA-N
Formula: C8H6F3NO
SMILES: CNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 189.13

Physical Properties

Property code	Value	Unit	Source
gf	-523.96	kJ/mol	Joback Method
hf	-653.77	kJ/mol	Joback Method
hfus	25.29	kJ/mol	Joback Method
hvap	48.39	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.464		Crippen Method
mcvol	116.680	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
tb	525.91	K	Joback Method
tc	720.06	K	Joback Method
tf	348.26	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.38	J/mol×K	525.91	Joback Method
cpg	267.74	J/mol×K	558.27	Joback Method
cpg	276.61	J/mol×K	590.63	Joback Method
cpg	285.01	J/mol×K	622.98	Joback Method
cpg	292.95	J/mol×K	655.34	Joback Method
cpg	300.43	J/mol×K	687.70	Joback Method
cpg	307.47	J/mol×K	720.06	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=U407256&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
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