Benzoic acid, 4-(trifluoroacetylamino)-

Inchi: InChI=1S/C9H6F3NO3/c10-9(11,12)8(16)13-6-3-1-5(2-4-6)7(14)15/h1-4H,(H,13,16)(H,14
InchiKey: TZDURDLECJWHJD-UHFFFAOYSA-N
Formula: C9H6F3NO3
SMILES: O=C(O)c1ccc(NC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 233.14
CAS: 404-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-759.18	kJ/mol	Joback Method
hf	-925.03	kJ/mol	Joback Method
hfus	26.93	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.886		Crippen Method
mcvol	138.210	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	681.65	K	Joback Method
tc	878.18	K	Joback Method
tf	447.66	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.15	J/mol×K	681.65	Joback Method
cpg	371.11	J/mol×K	714.41	Joback Method
cpg	378.45	J/mol×K	747.16	Joback Method
cpg	385.19	J/mol×K	779.92	Joback Method
cpg	391.40	J/mol×K	812.67	Joback Method
cpg	397.10	J/mol×K	845.43	Joback Method
cpg	402.33	J/mol×K	878.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C404262&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