«alpha»,«alpha»,«alpha»-trifluoro-p-toluic acid

Other names:	4-Trifluoromethylbenzoic acid
	p-Trifluoromethylbenzoic acid
	Benzoic acid, 4-(trifluoromethyl)-
Inchi:	InChI=1S/C8H5F3O2/c9-8(10,11)6-3-1-5(2-4-6)7(12)13/h1-4H,(H,12,13)
InchiKey:	SWKPKONEIZGROQ-UHFFFAOYSA-N
Formula:	C8H5F3O2
SMILES:	O=C(O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	190.12
CAS:	455-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-728.07	kJ/mol	Joback Method
hf	-845.28	kJ/mol	Joback Method
hfus	17.64	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.404		Crippen Method
mcvol	112.570	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	554.73	K	Joback Method
tc	745.16	K	Joback Method
tf	333.80	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.67	J/mol×K	554.73	Joback Method
cpg	273.20	J/mol×K	586.47	Joback Method
cpg	281.11	J/mol×K	618.21	Joback Method
cpg	288.45	J/mol×K	649.94	Joback Method
cpg	295.25	J/mol×K	681.68	Joback Method
cpg	301.53	J/mol×K	713.42	Joback Method

cpg	307.35	J/mol×K	745.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C455243&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

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