4-(Trifluoroacetyl)toluene

Inchi: InChI=1S/C9H7F3O/c1-6-2-4-7(5-3-6)8(13)9(10,11)12/h2-5H,1H3
InchiKey: DYILUJUELMWXAL-UHFFFAOYSA-N
Formula: C9H7F3O
SMILES: Cc1ccc(C(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 188.15
CAS: 394-59-2

Physical Properties

Property code	Value	Unit	Source
gf	-582.83	kJ/mol	Joback Method
hf	-713.69	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	41.56	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.740		Crippen Method
mcvol	120.790	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
tb	485.43	K	Joback Method
tc	685.09	K	Joback Method
tf	284.25	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.80	J/mol×K	485.43	Joback Method
cpg	273.51	J/mol×K	518.71	Joback Method
cpg	284.43	J/mol×K	551.98	Joback Method
cpg	294.60	J/mol×K	585.26	Joback Method
cpg	304.05	J/mol×K	618.54	Joback Method
cpg	312.82	J/mol×K	651.81	Joback Method
cpg	320.96	J/mol×K	685.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C394592&Units=SI

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