4-Trifluoromethylcinnamic acid

Other names: 2-Propenoic acid, 3-[4-(trifluoromethyl)phenyl]-
3-[4-(Trifluoromethyl)phenyl]-2-propenoic acid
p-(trifluoromethyl)cinnamic acid
Inchi: InChI=1S/C10H7F3O2/c11-10(12,13)8-4-1-7(2-5-8)3-6-9(14)15/h1-6H,(H,14,15)/b6-3+
InchiKey: ANRMAUMHJREENI-ZZXKWVIFSA-N
Formula: C10H7F3O2
SMILES: O=C(O)C=Cc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 216.16
CAS: 2062-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-631.01	kJ/mol	Joback Method
hf	-769.34	kJ/mol	Joback Method
hfus	23.02	kJ/mol	Joback Method
hvap	60.43	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.803		Crippen Method
mcvol	136.450	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
tb	604.65	K	Joback Method
tc	798.05	K	Joback Method
tf	351.26	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.10	J/mol×K	604.65	Joback Method
cpg	343.51	J/mol×K	636.88	Joback Method
cpg	352.23	J/mol×K	669.12	Joback Method
cpg	360.31	J/mol×K	701.35	Joback Method
cpg	367.79	J/mol×K	733.58	Joback Method
cpg	374.74	J/mol×K	765.82	Joback Method

cpg	381.19	J/mol×K	798.05	Joback Method

Sources

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=C2062262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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