2,3,5,6-Tetrafluoro-p-xylene

Inchi: InChI=1S/C8H6F4/c1-3-5(9)7(11)4(2)8(12)6(3)10/h1-2H3
InchiKey: IWKPBYPUIPVYNZ-UHFFFAOYSA-N
Formula: C8H6F4
SMILES: Cc1c(F)c(F)c(C)c(F)c1F
Mol. weight [g/mol]: 178.13
CAS: 703-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-698.50	kJ/mol	Joback Method
hf	-813.71	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	35.72	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.860		Crippen Method
mcvol	106.900	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	416.70	K	NIST Webbook
tc	605.68	K	Joback Method
tf	271.30	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.38	J/mol×K	431.10	Joback Method
cpg	221.67	J/mol×K	460.20	Joback Method
cpg	229.69	J/mol×K	489.29	Joback Method
cpg	237.42	J/mol×K	518.39	Joback Method
cpg	244.89	J/mol×K	547.48	Joback Method
cpg	252.08	J/mol×K	576.58	Joback Method
cpg	259.00	J/mol×K	605.68	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=C703877&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