3-CF3-C6H4-CCH

Inchi: InChI=1S/C9H5F3/c1-2-7-4-3-5-8(6-7)9(10,11)12/h1,3-6H
InchiKey: PAHXLHWOHJTWRU-UHFFFAOYSA-N
Formula: C9H5F3
SMILES: C#Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 170.13
CAS: 705-28-2

Physical Properties

Property code	Value	Unit	Source
affp	806.20	kJ/mol	NIST Webbook
basg	773.80	kJ/mol	NIST Webbook
gf	-230.84	kJ/mol	Joback Method
hf	-309.21	kJ/mol	Joback Method
hfus	17.52	kJ/mol	Joback Method
hvap	34.68	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.687		Crippen Method
mcvol	110.620	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	421.68	K	Joback Method
tc	624.59	K	Joback Method
tf	281.29	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.08	J/mol×K	421.68	Joback Method
cpg	226.50	J/mol×K	455.50	Joback Method
cpg	237.08	J/mol×K	489.32	Joback Method
cpg	246.87	J/mol×K	523.14	Joback Method
cpg	255.90	J/mol×K	556.95	Joback Method
cpg	264.24	J/mol×K	590.77	Joback Method
cpg	271.92	J/mol×K	624.59	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=C705282&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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

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