1-Ethynyl-3,5-bis(trifluoromethyl)benzene

Inchi: InChI=1S/C10H4F6/c1-2-6-3-7(9(11,12)13)5-8(4-6)10(14,15)16/h1,3-5H
InchiKey: MAHIBRPXUPUAIF-UHFFFAOYSA-N
Formula: C10H4F6
SMILES: C#Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 238.13
CAS: 88444-81-9

Physical Properties

Property code	Value	Unit	Source
gf	-813.64	kJ/mol	Joback Method
hf	-938.40	kJ/mol	Joback Method
hfus	21.55	kJ/mol	Joback Method
hvap	33.82	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.706		Crippen Method
mcvol	130.020	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	812.10		NIST Webbook
rinpol	812.10		NIST Webbook
tb	444.12	K	Joback Method
tc	627.55	K	Joback Method
tf	309.27	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.84	J/mol×K	444.12	Joback Method
cpg	294.31	J/mol×K	474.69	Joback Method
cpg	304.94	J/mol×K	505.26	Joback Method
cpg	314.76	J/mol×K	535.83	Joback Method
cpg	323.81	J/mol×K	566.40	Joback Method
cpg	332.16	J/mol×K	596.98	Joback Method
cpg	339.84	J/mol×K	627.55	Joback Method

Sources

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=C88444819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume