

4-(Trifluoromethyl)phenyl methanol, isopropyl ether

Inchi:	InChI=1S/C11H13F3O/c1-8(2)15-7-9-3-5-10(6-4-9)11(12,13)14/h3-6,8H,7H2,1-2H3
InchiKey:	LCONMZAIEAWMSG-UHFFFAOYSA-N
Formula:	C11H13F3O
SMILES:	CC(C)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	218.22

Physical Properties

Property code	Value	Unit	Source
gf	-544.51	kJ/mol	Joback Method
hf	-779.89	kJ/mol	Joback Method
hfus	17.39	kJ/mol	Joback Method
hvap	41.29	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.630		Crippen Method
mcvol	153.270	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1141.00		NIST Webbook
rinpol	1141.00		NIST Webbook
tb	499.30	K	Joback Method
tc	687.43	K	Joback Method
tf	264.09	K	Joback Method
vc	0.599	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.96	J/mol×K	499.30	Joback Method
cpg	368.54	J/mol×K	530.66	Joback Method
cpg	382.33	J/mol×K	562.01	Joback Method
cpg	395.34	J/mol×K	593.37	Joback Method
cpg	407.61	J/mol×K	624.72	Joback Method
cpg	419.16	J/mol×K	656.08	Joback Method
cpg	430.03	J/mol×K	687.43	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=U374435&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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