

4-(Trifluoromethyl)phenyl methanol, ethyl ether

Inchi:	InChI=1S/C10H11F3O/c1-2-14-7-8-3-5-9(6-4-8)10(11,12)13/h3-6H,2,7H2,1H3
InchiKey:	GDSWOTCSTHKKSB-UHFFFAOYSA-N
Formula:	C10H11F3O
SMILES:	CCOCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	204.19

Physical Properties

Property code	Value	Unit	Source
gf	-550.49	kJ/mol	Joback Method
hf	-753.97	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.242		Crippen Method
mcvol	139.180	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1093.00		NIST Webbook
tb	476.86	K	Joback Method
tc	663.03	K	Joback Method
tf	267.82	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.34	J/mol×K	476.86	Joback Method
cpg	322.73	J/mol×K	507.89	Joback Method
cpg	335.40	J/mol×K	538.92	Joback Method
cpg	347.37	J/mol×K	569.95	Joback Method
cpg	358.66	J/mol×K	600.97	Joback Method
cpg	369.29	J/mol×K	632.00	Joback Method
cpg	379.31	J/mol×K	663.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U374661&Units=SI

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
hvac:	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

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