4-(Trifluoromethyl)phenyl methanol, tert.-butyl ether

Inchi: InChI=1S/C12H15F3O/c1-11(2,3)16-8-9-4-6-10(7-5-9)12(13,14)15/h4-7H,8H2,1-3H3
InchiKey: DDYYKYXUNPEZCS-UHFFFAOYSA-N
Formula: C12H15F3O
SMILES: CC(C)(C)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 232.24

Physical Properties

Property code	Value	Unit	Source
gf	-530.81	kJ/mol	Joback Method
hf	-804.00	kJ/mol	Joback Method
hfus	16.09	kJ/mol	Joback Method
hvap	42.61	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.021		Crippen Method
mcvol	167.360	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
tb	519.39	K	Joback Method
tc	712.51	K	Joback Method
tf	292.78	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.98	J/mol×K	519.39	Joback Method
cpg	418.98	J/mol×K	551.58	Joback Method
cpg	433.98	J/mol×K	583.76	Joback Method
cpg	448.03	J/mol×K	615.95	Joback Method
cpg	461.18	J/mol×K	648.14	Joback Method
cpg	473.47	J/mol×K	680.33	Joback Method
cpg	484.96	J/mol×K	712.51	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=U374433&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume