4-(Trifluoromethyl)phenyl methanol, 3-methylbutyl ether

Inchi: InChI=1S/C13H17F3O/c1-10(2)7-8-17-9-11-3-5-12(6-4-11)13(14,15)16/h3-6,10H,7-9H2,1

InchiKey: ARECSLYCXPRNAF-UHFFFAOYSA-N

Formula: C13H17F3O

SMILES: CC(C)CCOCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 246.27

Physical Properties

Property code	Value	Unit	Source
gf	-527.67	kJ/mol	Joback Method
hf	-821.17	kJ/mol	Joback Method
hfus	22.57	kJ/mol	Joback Method
hvap	45.75	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.268		Crippen Method
mcvol	181.450	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	1336.00		NIST Webbook
rinpol	1336.00		NIST Webbook
tb	545.06	K	Joback Method
tc	729.04	K	Joback Method
tf	286.63	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.25	J/mol×K	545.06	Joback Method
cpg	464.16	J/mol×K	575.72	Joback Method
cpg	479.22	J/mol×K	606.39	Joback Method
cpg	493.46	J/mol×K	637.05	Joback Method
cpg	506.90	J/mol×K	667.72	Joback Method
cpg	519.58	J/mol×K	698.38	Joback Method
cpg	531.53	J/mol×K	729.04	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=U374431&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