4-(Trifluoromethyl)phenyl methanol, neopentyl ether

Inchi: InChI=1S/C13H17F3O/c1-12(2,3)9-17-8-10-4-6-11(7-5-10)13(14,15)16/h4-7H,8-9H2,1-3

InchiKey: SNLUEHIBOUEBIE-UHFFFAOYSA-N

Formula: C13H17F3O

SMILES: CC(C)(C)COCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 246.27

Physical Properties

Property code	Value	Unit	Source
gf	-522.39	kJ/mol	Joback Method
hf	-824.64	kJ/mol	Joback Method
hfus	18.68	kJ/mol	Joback Method
hvap	44.84	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.268		Crippen Method
mcvol	181.450	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1254.00		NIST Webbook
tb	542.27	K	Joback Method
tc	733.00	K	Joback Method
tf	304.05	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.96	J/mol×K	542.27	Joback Method
cpg	467.51	J/mol×K	574.06	Joback Method
cpg	483.04	J/mol×K	605.85	Joback Method
cpg	497.61	J/mol×K	637.63	Joback Method
cpg	511.28	J/mol×K	669.42	Joback Method
cpg	524.07	J/mol×K	701.21	Joback Method
cpg	536.06	J/mol×K	733.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U374432&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
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