

4-(Trifluoromethyl)phenyl methanol, 1-methylpropyl ether

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

Physical Properties

Property code	Value	Unit	Source
gf	-536.09	kJ/mol	Joback Method
hf	-800.53	kJ/mol	Joback Method
hfus	19.98	kJ/mol	Joback Method
hvap	43.52	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.021		Crippen Method
mcvol	167.360	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
tb	522.18	K	Joback Method
tc	708.20	K	Joback Method
tf	275.36	K	Joback Method
vc	0.654	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.24	J/mol×K	522.18	Joback Method
cpg	415.54	J/mol×K	553.18	Joback Method
cpg	430.01	J/mol×K	584.19	Joback Method
cpg	443.67	J/mol×K	615.19	Joback Method
cpg	456.57	J/mol×K	646.19	Joback Method
cpg	468.73	J/mol×K	677.19	Joback Method
cpg	480.17	J/mol×K	708.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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