4-(Trifluoromethyl)phenyl methanol, n-butyl ether

Inchi: InChI=1S/C12H15F3O/c1-2-3-8-16-9-10-4-6-11(7-5-10)12(13,14)15/h4-7H,2-3,8-9H2,1H

InchiKey: SFIBIHXUQBZIOG-UHFFFAOYSA-N

Formula: C12H15F3O

SMILES: CCCCOCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 232.24

Physical Properties

Property code	Value	Unit	Source
gf	-533.65	kJ/mol	Joback Method
hf	-795.25	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.022		Crippen Method
mcvol	167.360	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	1278.00		NIST Webbook
tb	522.62	K	Joback Method
tc	704.91	K	Joback Method
tf	290.36	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.00	J/mol×K	522.62	Joback Method
cpg	414.92	J/mol×K	553.00	Joback Method
cpg	429.06	J/mol×K	583.38	Joback Method
cpg	442.43	J/mol×K	613.76	Joback Method
cpg	455.07	J/mol×K	644.15	Joback Method
cpg	467.01	J/mol×K	674.53	Joback Method
cpg	478.27	J/mol×K	704.91	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=U374434&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