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

Inchi: InChI=1S/C13H17F3O/c1-2-3-4-9-17-10-11-5-7-12(8-6-11)13(14,15)16/h5-8H,2-4,9-10H
InchiKey: RYOMOXNDDLHZJM-UHFFFAOYSA-N
Formula: C13H17F3O
SMILES: CCCCCOCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 246.27

Physical Properties

Property code	Value	Unit	Source
gf	-525.23	kJ/mol	Joback Method
hf	-815.89	kJ/mol	Joback Method
hfus	26.09	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.412		Crippen Method
mcvol	181.450	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1375.00		NIST Webbook
tb	545.50	K	Joback Method
tc	725.96	K	Joback Method
tf	301.63	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.97	J/mol×K	545.50	Joback Method
cpg	463.52	J/mol×K	575.58	Joback Method
cpg	478.25	J/mol×K	605.65	Joback Method
cpg	492.20	J/mol×K	635.73	Joback Method
cpg	505.39	J/mol×K	665.80	Joback Method
cpg	517.86	J/mol×K	695.88	Joback Method
cpg	529.62	J/mol×K	725.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374430&Units=SI
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

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