2,4,5-Trifluorobenzyl alcohol, n-pentyl ether

Inchi: InChI=1S/C12H15F3O/c1-2-3-4-5-16-8-9-6-11(14)12(15)7-10(9)13/h6-7H,2-5,8H2,1H3
InchiKey: QOGDMLVMSSJTHS-UHFFFAOYSA-N
Formula: C12H15F3O
SMILES: CCCCCOCc1cc(F)c(F)cc1F
Mol. weight [g/mol]: 232.24

Physical Properties

Property code	Value	Unit	Source
gf	-555.75	kJ/mol	Joback Method
hf	-809.44	kJ/mol	Joback Method
hfus	30.14	kJ/mol	Joback Method
hvap	46.53	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.811		Crippen Method
mcvol	167.360	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1328.00		NIST Webbook
tb	535.81	K	Joback Method
tc	710.43	K	Joback Method
tf	312.98	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.58	J/mol×K	535.81	Joback Method
cpg	411.01	J/mol×K	564.91	Joback Method
cpg	423.90	J/mol×K	594.02	Joback Method
cpg	436.26	J/mol×K	623.12	Joback Method
cpg	448.07	J/mol×K	652.22	Joback Method
cpg	459.37	J/mol×K	681.33	Joback Method
cpg	470.14	J/mol×K	710.43	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=U375252&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