

3,4,5-Trifluorobenzyl alcohol, n-propyl ether

Inchi:	InChI=1S/C10H11F3O/c1-2-3-14-6-7-4-8(11)10(13)9(12)5-7/h4-5H,2-3,6H2,1H3
InchiKey:	QKDKAJXSSJITEJ-UHFFFAOYSA-N
Formula:	C10H11F3O
SMILES:	CCCOc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]:	204.19

Physical Properties

Property code	Value	Unit	Source
gf	-572.59	kJ/mol	Joback Method
hf	-768.16	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	42.08	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.030		Crippen Method
mcvol	139.180	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinsol	1160.00		NIST Webbook
tb	490.05	K	Joback Method
tc	667.77	K	Joback Method
tf	290.44	K	Joback Method
vc	0.559	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.37	J/mol×K	490.05	Joback Method
cpg	319.01	J/mol×K	519.67	Joback Method
cpg	330.20	J/mol×K	549.29	Joback Method
cpg	340.95	J/mol×K	578.91	Joback Method
cpg	351.25	J/mol×K	608.53	Joback Method
cpg	361.12	J/mol×K	638.15	Joback Method
cpg	370.54	J/mol×K	667.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375248&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

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

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