1-(4-Fluorophenyl)-2-methyl-2-propanol

Inchi: InChI=1S/C10H13FO/c1-10(2,12)7-8-3-5-9(11)6-4-8/h3-6,12H,7H2,1-2H3
InchiKey: DWRIANGNJXQAAT-UHFFFAOYSA-N
Formula: C10H13FO
SMILES: CC(C)(O)Cc1ccc(F)cc1
Mol. weight [g/mol]: 168.21
CAS: 2928-17-8

Physical Properties

Property code	Value	Unit	Source
gf	-192.69	kJ/mol	Joback Method
hf	-381.76	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	55.36	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.139		Crippen Method
mcvol	135.640	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	548.08	K	Joback Method
tc	743.44	K	Joback Method
tf	305.23	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.13	J/mol×K	548.08	Joback Method
cpg	335.53	J/mol×K	580.64	Joback Method
cpg	347.15	J/mol×K	613.20	Joback Method
cpg	358.05	J/mol×K	645.76	Joback Method
cpg	368.26	J/mol×K	678.32	Joback Method
cpg	377.83	J/mol×K	710.88	Joback Method
cpg	386.79	J/mol×K	743.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2928178&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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