2,6-Difluoro-«alpha»-methylbenzyl alcohol, acetate

Inchi: InChI=1S/C10H10F2O2/c1-6(14-7(2)13)10-8(11)4-3-5-9(10)12/h3-6H,1-2H3
InchiKey: MZLPMTQUTDNLHM-UHFFFAOYSA-N
Formula: C10H10F2O2
SMILES: CC(=O)OC(C)c1c(F)cccc1F
Mol. weight [g/mol]: 200.18

Physical Properties

Property code	Value	Unit	Source
gf	-499.51	kJ/mol	Joback Method
hf	-678.44	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	48.59	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.589		Crippen Method
mcvol	138.980	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	1195.00		NIST Webbook
tb	539.23	K	Joback Method
tc	737.94	K	Joback Method
tf	312.26	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.87	J/mol×K	539.23	Joback Method
cpg	328.88	J/mol×K	572.35	Joback Method
cpg	340.29	J/mol×K	605.47	Joback Method
cpg	351.12	J/mol×K	638.59	Joback Method
cpg	361.36	J/mol×K	671.70	Joback Method
cpg	371.03	J/mol×K	704.82	Joback Method
cpg	380.13	J/mol×K	737.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368769&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume