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

Inchi: InChI=1S/C15H12F2O2/c1-10(14-12(16)8-5-9-13(14)17)19-15(18)11-6-3-2-4-7-11/h2-10
InchiKey: JFYUZPRGWAUQJN-UHFFFAOYSA-N
Formula: C15H12F2O2
SMILES: CC(OC(=O)c1ccccc1)c1c(F)cccc1F
Mol. weight [g/mol]: 262.25

Physical Properties

Property code	Value	Unit	Source
gf	-345.00	kJ/mol	Joback Method
hf	-545.11	kJ/mol	Joback Method
hfus	27.33	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.883		Crippen Method
mcvol	185.670	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1786.00		NIST Webbook
tb	680.31	K	Joback Method
tc	903.22	K	Joback Method
tf	395.03	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.37	J/mol×K	680.31	Joback Method
cpg	495.61	J/mol×K	717.46	Joback Method
cpg	508.80	J/mol×K	754.61	Joback Method
cpg	520.99	J/mol×K	791.77	Joback Method
cpg	532.20	J/mol×K	828.92	Joback Method
cpg	542.47	J/mol×K	866.07	Joback Method
cpg	551.84	J/mol×K	903.22	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=U368770&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