2,5-Difluorobenzyl alcohol, n-butyl

Inchi: InChI=1S/C11H14F2O/c1-2-3-6-14-8-9-7-10(12)4-5-11(9)13/h4-5,7H,2-3,6,8H2,1H3
InchiKey: KKYCXJVPKNTKAB-UHFFFAOYSA-N
Formula: C11H14F2O
SMILES: CCCCOCc1cc(F)ccc1F
Mol. weight [g/mol]: 200.23

Physical Properties

Property code	Value	Unit	Source
gf	-359.73	kJ/mol	Joback Method
hf	-581.22	kJ/mol	Joback Method
hfus	24.86	kJ/mol	Joback Method
hvap	44.46	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.281		Crippen Method
mcvol	151.500	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1252.00		NIST Webbook
tb	508.68	K	Joback Method
tc	692.23	K	Joback Method
tf	288.60	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.96	J/mol×K	508.68	Joback Method
cpg	356.47	J/mol×K	539.27	Joback Method
cpg	369.40	J/mol×K	569.86	Joback Method
cpg	381.76	J/mol×K	600.46	Joback Method
cpg	393.56	J/mol×K	631.05	Joback Method
cpg	404.80	J/mol×K	661.64	Joback Method
cpg	415.50	J/mol×K	692.23	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=U378164&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