2,5-Difluorobenzyl alcohol, n-pentyl

Inchi: InChI=1S/C12H16F2O/c1-2-3-4-7-15-9-10-8-11(13)5-6-12(10)14/h5-6,8H,2-4,7,9H2,1H3
InchiKey: GUXXEZLCRMKMBH-UHFFFAOYSA-N
Formula: C12H16F2O
SMILES: CCCCCOCc1cc(F)ccc1F
Mol. weight [g/mol]: 214.25

Physical Properties

Property code	Value	Unit	Source
gf	-351.31	kJ/mol	Joback Method
hf	-601.86	kJ/mol	Joback Method
hfus	27.45	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.672		Crippen Method
mcvol	165.590	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook
tb	531.56	K	Joback Method
tc	713.21	K	Joback Method
tf	299.87	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.12	J/mol×K	531.56	Joback Method
cpg	403.46	J/mol×K	561.84	Joback Method
cpg	417.18	J/mol×K	592.11	Joback Method
cpg	430.29	J/mol×K	622.39	Joback Method
cpg	442.79	J/mol×K	652.66	Joback Method
cpg	454.69	J/mol×K	682.94	Joback Method
cpg	466.02	J/mol×K	713.21	Joback Method

Sources

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=U378168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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