2,5-Difluorobenzyl alcohol, neopentyl ether

Inchi: InChI=1S/C12H16F2O/c1-12(2,3)8-15-7-9-6-10(13)4-5-11(9)14/h4-6H,7-8H2,1-3H3
InchiKey: XCTDKTCMCLWQNA-UHFFFAOYSA-N
Formula: C12H16F2O
SMILES: CC(C)(C)COCc1cc(F)ccc1F
Mol. weight [g/mol]: 214.25

Physical Properties

Property code	Value	Unit	Source
gf	-348.47	kJ/mol	Joback Method
hf	-610.61	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	45.39	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.527		Crippen Method
mcvol	165.590	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1228.00		NIST Webbook
rinpol	1228.00		NIST Webbook
tb	528.33	K	Joback Method
tc	720.61	K	Joback Method
tf	302.29	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.22	J/mol×K	528.33	Joback Method
cpg	407.54	J/mol×K	560.38	Joback Method
cpg	422.05	J/mol×K	592.42	Joback Method
cpg	435.79	J/mol×K	624.47	Joback Method
cpg	448.77	J/mol×K	656.52	Joback Method
cpg	461.04	J/mol×K	688.56	Joback Method
cpg	472.60	J/mol×K	720.61	Joback Method

Sources

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=U378169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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