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

Inchi: InChI=1S/C8H8F2O/c1-5(11)8-6(9)3-2-4-7(8)10/h2-5,11H,1H3
InchiKey: SIYWDKQSSDBLOA-UHFFFAOYSA-N
Formula: C8H8F2O
SMILES: CC(O)c1c(F)cccc1F
Mol. weight [g/mol]: 158.15
CAS: 87327-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-419.25	kJ/mol	Joback Method
hf	-544.59	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	51.66	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.018		Crippen Method
mcvol	109.230	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
tb	509.36	K	Joback Method
tc	694.19	K	Joback Method
tf	278.38	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.03	J/mol×K	509.36	Joback Method
cpg	249.34	J/mol×K	540.17	Joback Method
cpg	258.18	J/mol×K	570.97	Joback Method
cpg	266.58	J/mol×K	601.78	Joback Method
cpg	274.53	J/mol×K	632.58	Joback Method
cpg	282.07	J/mol×K	663.39	Joback Method
cpg	289.19	J/mol×K	694.19	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=C87327659&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