2,4-Difluorobenzyl alcohol

Other names: Benzenemethanol, 2,4-difluoro-
Inchi: InChI=1S/C7H6F2O/c8-6-2-1-5(4-10)7(9)3-6/h1-3,10H,4H2
InchiKey: NIJZBWHOHNWJBX-UHFFFAOYSA-N
Formula: C7H6F2O
SMILES: OCc1ccc(F)cc1F
Mol. weight [g/mol]: 144.12
CAS: 56456-47-4

Physical Properties

Property code	Value	Unit	Source
gf	-425.23	kJ/mol	Joback Method
hf	-518.67	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	49.82	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.457		Crippen Method
mcvol	95.140	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	486.92	K	Joback Method
tc	669.83	K	Joback Method
tf	282.11	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.74	J/mol×K	486.92	Joback Method
cpg	206.72	J/mol×K	517.41	Joback Method
cpg	214.31	J/mol×K	547.89	Joback Method
cpg	221.52	J/mol×K	578.38	Joback Method
cpg	228.37	J/mol×K	608.86	Joback Method
cpg	234.86	J/mol×K	639.35	Joback Method
cpg	241.00	J/mol×K	669.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56456474&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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