3,4-Difluorobenzylamine

Other names:	Benzenemethanamine, 3,4-difluoro-
Inchi:	InChI=1S/C7H7F2N/c8-6-2-1-5(4-10)3-7(6)9/h1-3H,4,10H2
InchiKey:	PHLZUDXEBCQHKM-UHFFFAOYSA-N
Formula:	C7H7F2N
SMILES:	NCc1ccc(F)c(F)c1
Mol. weight [g/mol]:	143.13
CAS:	72235-53-1

Physical Properties

Property code	Value	Unit	Source
gf	-221.96	kJ/mol	Joback Method
hf	-332.65	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	43.78	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.424		Crippen Method
mcvol	99.250	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	467.27	K	Joback Method
tc	672.73	K	Joback Method
tf	304.55	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.90	J/mol×K	467.27	Joback Method
cpg	214.68	J/mol×K	501.51	Joback Method
cpg	223.94	J/mol×K	535.76	Joback Method
cpg	232.68	J/mol×K	570.00	Joback Method
cpg	240.93	J/mol×K	604.24	Joback Method
cpg	248.71	J/mol×K	638.49	Joback Method
cpg	256.02	J/mol×K	672.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72235531&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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