N,N-Bis(2-hydroxyethyl)-m-fluoroaniline

Inchi: InChI=1S/C10H14FNO2/c11-9-2-1-3-10(8-9)12(4-6-13)5-7-14/h1-3,8,13-14H,4-7H2
InchiKey: GFXQBWUWIQBIKN-UHFFFAOYSA-N
Formula: C10H14FNO2
SMILES: OCCN(CCO)c1cccc(F)c1
Mol. weight [g/mol]: 199.22
CAS: 323-60-4

Physical Properties

Property code	Value	Unit	Source
gf	-221.57	kJ/mol	Joback Method
hf	-457.71	kJ/mol	Joback Method
hfus	29.59	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	0.617		Crippen Method
mcvol	151.490	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	655.93	K	Joback Method
tc	832.25	K	Joback Method
tf	396.10	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.84	J/mol×K	655.93	Joback Method
cpg	416.99	J/mol×K	685.32	Joback Method
cpg	426.59	J/mol×K	714.70	Joback Method
cpg	435.66	J/mol×K	744.09	Joback Method
cpg	444.23	J/mol×K	773.47	Joback Method
cpg	452.31	J/mol×K	802.86	Joback Method
cpg	459.94	J/mol×K	832.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.50 ± 0.50	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C323604&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume