4-fluoro-«alpha»-methylbenzylamine

Inchi: InChI=1S/C8H10FN/c1-6(10)7-2-4-8(9)5-3-7/h2-6H,10H2,1H3
InchiKey: QGCLEUGNYRXBMZ-UHFFFAOYSA-N
Formula: C8H10FN
SMILES: CC(N)c1ccc(F)cc1
Mol. weight [g/mol]: 139.17
CAS: 403-40-7

Physical Properties

Property code	Value	Unit	Source
gf	-11.54	kJ/mol	Joback Method
hf	-150.99	kJ/mol	Joback Method
hfus	14.88	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.845		Crippen Method
mcvol	111.570	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	485.46	K	Joback Method
tc	702.91	K	Joback Method
tf	287.71	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.33	J/mol×K	485.46	Joback Method
cpg	249.65	J/mol×K	521.70	Joback Method
cpg	261.24	J/mol×K	557.94	Joback Method
cpg	272.11	J/mol×K	594.19	Joback Method
cpg	282.30	J/mol×K	630.43	Joback Method
cpg	291.85	J/mol×K	666.67	Joback Method
cpg	300.76	J/mol×K	702.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C403407&Units=SI

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