

Benzylamine, o-fluoro-n-methyl-n-2-propynyl-

Inchi:	InChI=1S/C11H12FN/c1-3-8-13(2)9-10-6-4-5-7-11(10)12/h1,4-7H,8-9H2,2H3
InchiKey:	TZJVMCHRLXKQS-UHFFFAOYSA-N
Formula:	C11H12FN
SMILES:	C#CCN(C)Cc1ccccc1F
Mol. weight [g/mol]:	177.22
CAS:	709-54-6

Physical Properties

Property code	Value	Unit	Source
gf	283.56	kJ/mol	Joback Method
hf	118.01	kJ/mol	Joback Method
hfus	26.97	kJ/mol	Joback Method
hvap	44.10	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	1.891		Crippen Method
mcvol	145.240	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
tb	484.57	K	Joback Method
tc	688.73	K	Joback Method
tf	332.70	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.71	J/molxK	484.57	Joback Method
cpg	323.13	J/molxK	518.60	Joback Method
cpg	336.66	J/molxK	552.62	Joback Method
cpg	349.35	J/molxK	586.65	Joback Method
cpg	361.25	J/molxK	620.67	Joback Method
cpg	372.39	J/molxK	654.70	Joback Method
cpg	382.82	J/molxK	688.73	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=C709546&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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