Benzamide, n-(3-methylphenyl)-3-fluoro-

Inchi: InChI=1S/C14H12FNO/c1-10-4-2-7-13(8-10)16-14(17)11-5-3-6-12(15)9-11/h2-9H,1H3,(H
InchiKey: JXURCZBELJVDNC-UHFFFAOYSA-N
Formula: C14H12FNO
SMILES: Cc1cccc(NC(=O)c2cccc(F)c2)c1
Mol. weight [g/mol]: 229.25

Physical Properties

Property code	Value	Unit	Source
hf	-227.20	kJ/mol	Cheméo Relay (1.0)
hfus	29.10	kJ/mol	Joback Method
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-4.31		Cheméo Relay (1.0)
logp	3.386		Crippen Method
mcvol	173.920	ml/mol	McGowan Method
rinpol	1988.00		NIST Webbook
tb	610.85	K	Cheméo Relay (1.0)
tc	906.15	K	Cheméo Relay (1.0)
tf	383.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.17	J/mol×K	686.35	Joback Method
cpg	461.07	J/mol×K	725.40	Joback Method
cpg	473.88	J/mol×K	764.45	Joback Method
cpg	485.66	J/mol×K	803.49	Joback Method
cpg	496.48	J/mol×K	842.54	Joback Method
cpg	506.39	J/mol×K	881.59	Joback Method
cpg	515.44	J/mol×K	920.64	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307164&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point