Benzamide, N-(3-methylphenyl)-2,6-difluoro-

Inchi: InChI=1S/C14H11F2NO/c1-9-4-2-5-10(8-9)17-14(18)13-11(15)6-3-7-12(13)16/h2-8H,1H3
InchiKey: GLJNSSJUIBRIQJ-UHFFFAOYSA-N
Formula: C14H11F2NO
SMILES: Cc1cccc(NC(=O)c2c(F)cccc2F)c1
Mol. weight [g/mol]: 247.24

Physical Properties

Property code	Value	Unit	Source
gf	-166.22	kJ/mol	Joback Method
hf	-344.97	kJ/mol	Joback Method
hfus	31.79	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.526		Crippen Method
mcvol	175.690	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1959.00		NIST Webbook
tb	690.60	K	Joback Method
tc	915.42	K	Joback Method
tf	441.71	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.98	J/mol×K	690.60	Joback Method
cpg	467.03	J/mol×K	728.07	Joback Method
cpg	479.12	J/mol×K	765.54	Joback Method
cpg	490.27	J/mol×K	803.01	Joback Method
cpg	500.55	J/mol×K	840.48	Joback Method
cpg	509.98	J/mol×K	877.95	Joback Method
cpg	518.63	J/mol×K	915.42	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=U307428&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume