Benzamide, 2-trifluoromethyl-5-fluoro-N-butyl-

Inchi: InChI=1S/C12H13F4NO/c1-2-3-6-17-11(18)9-7-8(13)4-5-10(9)12(14,15)16/h4-5,7H,2-3,6
InchiKey: WEMKHYPGWLQWOO-UHFFFAOYSA-N
Formula: C12H13F4NO
SMILES: CCCCNC(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]: 263.23

Physical Properties

Property code	Value	Unit	Source
gf	-672.62	kJ/mol	Joback Method
hf	-929.72	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	54.52	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.374		Crippen Method
mcvol	174.810	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook
tb	608.49	K	Joback Method
tc	794.47	K	Joback Method
tf	383.83	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.87	J/mol×K	608.49	Joback Method
cpg	467.71	J/mol×K	639.49	Joback Method
cpg	479.77	J/mol×K	670.48	Joback Method
cpg	491.09	J/mol×K	701.48	Joback Method
cpg	501.71	J/mol×K	732.47	Joback Method
cpg	511.67	J/mol×K	763.47	Joback Method
cpg	520.99	J/mol×K	794.47	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=U407676&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