Benzamide, 3-(trifluoromethyl)-N-(3-methylbutyl)-

Inchi: InChI=1S/C13H16F3NO/c1-9(2)6-7-17-12(18)10-4-3-5-11(8-10)13(14,15)16/h3-5,8-9H,6-

InchiKey: PNWRTYLJSNYYSV-UHFFFAOYSA-N

Formula: C13H16F3NO

SMILES: CC(C)CCNC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 259.27

Physical Properties

Property code	Value	Unit	Source
gf	-462.20	kJ/mol	Joback Method
hf	-748.06	kJ/mol	Joback Method
hfus	28.08	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.481		Crippen Method
mcvol	187.130	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	626.68	K	Joback Method
tc	820.96	K	Joback Method
tf	366.99	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.70	J/mol×K	626.68	Joback Method
cpg	512.16	J/mol×K	659.06	Joback Method
cpg	525.69	J/mol×K	691.44	Joback Method
cpg	538.34	J/mol×K	723.82	Joback Method
cpg	550.17	J/mol×K	756.20	Joback Method
cpg	561.23	J/mol×K	788.58	Joback Method
cpg	571.55	J/mol×K	820.96	Joback Method

Sources

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=U407168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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