Benzamide, 2,5-di(trifluoromethyl)-N-isobutyl-

Inchi: InChI=1S/C13H13F6NO/c1-7(2)6-20-11(21)9-5-8(12(14,15)16)3-4-10(9)13(17,18)19/h3-5
InchiKey: VETXVKNVUCBBJN-UHFFFAOYSA-N
Formula: C13H13F6NO
SMILES: CC(C)CNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 313.24

Physical Properties

Property code	Value	Unit	Source
gf	-1053.42	kJ/mol	Joback Method
hf	-1356.61	kJ/mol	Joback Method
hfus	29.52	kJ/mol	Joback Method
hvap	53.43	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.110		Crippen Method
mcvol	192.440	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	626.24	K	Joback Method
tc	807.85	K	Joback Method
tf	383.70	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.58	J/mol×K	626.24	Joback Method
cpg	537.61	J/mol×K	656.51	Joback Method
cpg	549.79	J/mol×K	686.78	Joback Method
cpg	561.15	J/mol×K	717.05	Joback Method
cpg	571.75	J/mol×K	747.32	Joback Method
cpg	581.64	J/mol×K	777.58	Joback Method
cpg	590.87	J/mol×K	807.85	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=U407917&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