Benzamide, 2,5-di(trifluoromethyl)-N-3-methylbutyl-

Inchi: InChI=1S/C14H15F6NO/c1-8(2)5-6-21-12(22)10-7-9(13(15,16)17)3-4-11(10)14(18,19)20

InchiKey: CPJVYJWOQOCYKV-UHFFFAOYSA-N

Formula: C14H15F6NO

SMILES: CC(C)CCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 327.27

Physical Properties

Property code	Value	Unit	Source
gf	-1045.00	kJ/mol	Joback Method
hf	-1377.25	kJ/mol	Joback Method
hfus	32.11	kJ/mol	Joback Method
hvap	55.66	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.500		Crippen Method
mcvol	206.530	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	649.12	K	Joback Method
tc	829.50	K	Joback Method
tf	394.97	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.60	J/mol×K	649.12	Joback Method
cpg	589.06	J/mol×K	679.18	Joback Method
cpg	601.65	J/mol×K	709.25	Joback Method
cpg	613.42	J/mol×K	739.31	Joback Method
cpg	624.43	J/mol×K	769.37	Joback Method
cpg	634.72	J/mol×K	799.44	Joback Method
cpg	644.34	J/mol×K	829.50	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=U407919&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