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

Inchi: InChI=1S/C12H14F3NO/c1-8(2)7-16-11(17)9-5-3-4-6-10(9)12(13,14)15/h3-6,8H,7H2,1-2
InchiKey: QSFAOLWJYNHKEP-UHFFFAOYSA-N
Formula: C12H14F3NO
SMILES: CC(C)CNC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 245.24

Physical Properties

Property code	Value	Unit	Source
gf	-470.62	kJ/mol	Joback Method
hf	-727.42	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	54.29	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.091		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1550.00		NIST Webbook
tb	603.80	K	Joback Method
tc	800.52	K	Joback Method
tf	355.72	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.67	J/mol×K	603.80	Joback Method
cpg	461.64	J/mol×K	636.59	Joback Method
cpg	474.69	J/mol×K	669.37	Joback Method
cpg	486.88	J/mol×K	702.16	Joback Method
cpg	498.25	J/mol×K	734.95	Joback Method
cpg	508.85	J/mol×K	767.74	Joback Method
cpg	518.73	J/mol×K	800.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407185&Units=SI
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

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