3'-Trifluoromethylisobutyranilide

Inchi: InChI=1S/C11H12F3NO/c1-7(2)10(16)15-9-5-3-4-8(6-9)11(12,13)14/h3-7H,1-2H3,(H,15,
InchiKey: GETMKVRSDFVVHL-UHFFFAOYSA-N
Formula: C11H12F3NO
SMILES: CC(C)C(=O)Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 231.21
CAS: 1939-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-479.04	kJ/mol	Joback Method
hf	-706.78	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.300		Crippen Method
mcvol	158.950	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
tb	580.92	K	Joback Method
tc	780.34	K	Joback Method
tf	344.45	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.11	J/mol×K	580.92	Joback Method
cpg	412.51	J/mol×K	614.16	Joback Method
cpg	425.01	J/mol×K	647.39	Joback Method
cpg	436.67	J/mol×K	680.63	Joback Method
cpg	447.51	J/mol×K	713.87	Joback Method
cpg	457.60	J/mol×K	747.10	Joback Method
cpg	466.98	J/mol×K	780.34	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=C1939271&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume