3'-Trifluoromethyl-2,2-dimethylvaleranilide

Inchi: InChI=1S/C14H18F3NO/c1-4-8-13(2,3)12(19)18-11-7-5-6-10(9-11)14(15,16)17/h5-7,9H,4
InchiKey: JZGSGKPJMMYYGT-UHFFFAOYSA-N
Formula: C14H18F3NO
SMILES: CCCC(C)(C)C(=O)Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 273.29
CAS: 2300-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-448.50	kJ/mol	Joback Method
hf	-772.17	kJ/mol	Joback Method
hfus	26.78	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.470		Crippen Method
mcvol	201.220	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
tb	646.77	K	Joback Method
tc	845.04	K	Joback Method
tf	395.68	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.61	J/mol×K	646.77	Joback Method
cpg	566.76	J/mol×K	679.82	Joback Method
cpg	580.88	J/mol×K	712.86	Joback Method
cpg	594.02	J/mol×K	745.91	Joback Method
cpg	606.27	J/mol×K	778.95	Joback Method
cpg	617.67	J/mol×K	812.00	Joback Method
cpg	628.32	J/mol×K	845.04	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=C2300870&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