3'-Trifluoromethyl-2-phenylacetanilide

Inchi: InChI=1S/C15H12F3NO/c16-15(17,18)12-7-4-8-13(10-12)19-14(20)9-11-5-2-1-3-6-11/h1
InchiKey: AWZJXXWDKOAELM-UHFFFAOYSA-N
Formula: C15H12F3NO
SMILES: O=C(Cc1ccccc1)Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 279.26
CAS: 1939-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-330.51	kJ/mol	Joback Method
hf	-547.53	kJ/mol	Joback Method
hfus	30.82	kJ/mol	Joback Method
hvap	63.63	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.887		Crippen Method
mcvol	191.550	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
tb	699.56	K	Joback Method
tc	921.09	K	Joback Method
tf	430.95	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.57	J/mol×K	699.56	Joback Method
cpg	532.17	J/mol×K	736.48	Joback Method
cpg	544.64	J/mol×K	773.40	Joback Method
cpg	556.08	J/mol×K	810.32	Joback Method
cpg	566.56	J/mol×K	847.24	Joback Method
cpg	576.18	J/mol×K	884.17	Joback Method
cpg	585.02	J/mol×K	921.09	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=C1939215&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