3'-Trifluoromethyl-o-toluanilide

Inchi: InChI=1S/C15H12F3NO/c1-10-5-2-3-8-13(10)14(20)19-12-7-4-6-11(9-12)15(16,17)18/h2
InchiKey: VNBKPVJBSIXIJX-UHFFFAOYSA-N
Formula: C15H12F3NO
SMILES: Cc1ccccc1C(=O)Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 279.26
CAS: 1939-22-6

Physical Properties

Property code	Value	Unit	Source
gf	-340.14	kJ/mol	Joback Method
hf	-559.00	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	64.30	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.266		Crippen Method
mcvol	191.550	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
tb	704.54	K	Joback Method
tc	926.89	K	Joback Method
tf	443.47	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.43	J/mol×K	704.54	Joback Method
cpg	530.86	J/mol×K	741.60	Joback Method
cpg	543.20	J/mol×K	778.66	Joback Method
cpg	554.54	J/mol×K	815.71	Joback Method
cpg	564.94	J/mol×K	852.77	Joback Method
cpg	574.50	J/mol×K	889.83	Joback Method
cpg	583.28	J/mol×K	926.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1939226&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume