3'-Trifluoromethylcyclopentanecarboxanilide

Inchi: InChI=1S/C13H14F3NO/c14-13(15,16)10-6-3-7-11(8-10)17-12(18)9-4-1-2-5-9/h3,6-9H,1-
InchiKey: PPEXRKPFMAVBPF-UHFFFAOYSA-N
Formula: C13H14F3NO
SMILES: O=C(Nc1cccc(C(F)(F)F)c1)C1CCCC1
Mol. weight [g/mol]: 257.25
CAS: 13691-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-423.21	kJ/mol	Joback Method
hf	-682.30	kJ/mol	Joback Method
hfus	25.54	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.834		Crippen Method
mcvol	176.270	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
tb	642.40	K	Joback Method
tc	858.28	K	Joback Method
tf	392.89	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.17	J/mol×K	642.40	Joback Method
cpg	502.18	J/mol×K	678.38	Joback Method
cpg	516.97	J/mol×K	714.36	Joback Method
cpg	530.62	J/mol×K	750.34	Joback Method
cpg	543.22	J/mol×K	786.32	Joback Method
cpg	554.83	J/mol×K	822.30	Joback Method
cpg	565.53	J/mol×K	858.28	Joback Method

Sources

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=C13691844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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