Benzamide, N-(3-chlorophenyl)-4-trifluoromethyl-

Inchi: InChI=1S/C14H9ClF3NO/c15-11-2-1-3-12(8-11)19-13(20)9-4-6-10(7-5-9)14(16,17)18/h1-

InchiKey: VDNNPBHKNGRCFB-UHFFFAOYSA-N

Formula: C14H9ClF3NO

SMILES: O=C(Nc1cccc(Cl)c1)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 299.68

Physical Properties

Property code	Value	Unit	Source
gf	-360.49	kJ/mol	Joback Method
hf	-554.10	kJ/mol	Joback Method
hfus	32.04	kJ/mol	Joback Method
hvap	66.45	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.611		Crippen Method
mcvol	189.700	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	719.09	K	Joback Method
tc	948.18	K	Joback Method
tf	462.12	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.70	J/mol×K	719.09	Joback Method
cpg	501.44	J/mol×K	757.27	Joback Method
cpg	512.14	J/mol×K	795.45	Joback Method
cpg	521.89	J/mol×K	833.64	Joback Method
cpg	530.76	J/mol×K	871.82	Joback Method
cpg	538.86	J/mol×K	910.00	Joback Method
cpg	546.25	J/mol×K	948.18	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=U307248&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume