

o-(trifluoromethyl)benzamide

Inchi:	InChI=1S/C8H6F3NO/c9-8(10,11)6-4-2-1-3-5(6)7(12)13/h1-4H,(H2,12,13)
InchiKey:	QBAYIBZITZBSFO-UHFFFAOYSA-N
Formula:	C8H6F3NO
SMILES:	NC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]:	189.13
CAS:	360-64-5

Physical Properties

Property code	Value	Unit	Source
gf	-524.80	kJ/mol	Joback Method
hf	-659.26	kJ/mol	Joback Method
hfus	18.75	kJ/mol	Joback Method
hvap	49.98	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	1.804		Crippen Method
mcvol	116.680	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	535.08	K	Joback Method
tc	748.18	K	Joback Method
tf	356.24	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.67	J/mol×K	535.08	Joback Method
cpg	282.12	J/mol×K	570.60	Joback Method
cpg	291.77	J/mol×K	606.11	Joback Method
cpg	300.65	J/mol×K	641.63	Joback Method
cpg	308.81	J/mol×K	677.15	Joback Method
cpg	316.31	J/mol×K	712.67	Joback Method
cpg	323.18	J/mol×K	748.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C360645&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

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

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