

4-Trifluoromethylbenzhydrazide

Other names:	4-Trifluoromethylbenzoic acid hydrazide Benzoic acid, 4-(trifluoromethyl)-, hydrazide
Inchi:	InChI=1S/C8H7F3N2O/c9-8(10,11)6-3-1-5(2-4-6)7(14)13-12/h1-4H,12H2,(H,13,14)
InchiKey:	GKBDXTNCBPZMFX-UHFFFAOYSA-N
Formula:	C8H7F3N2O
SMILES:	NNC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	204.15
CAS:	339-59-3

Physical Properties

Property code	Value	Unit	Source
gf	-435.41	kJ/mol	Joback Method
hf	-605.79	kJ/mol	Joback Method
hfus	23.85	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	1.309		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	585.25	K	Joback Method
tc	798.31	K	Joback Method
tf	408.90	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.04	J/mol×K	585.25	Joback Method
cpg	325.39	J/mol×K	620.76	Joback Method
cpg	334.93	J/mol×K	656.27	Joback Method
cpg	343.70	J/mol×K	691.78	Joback Method
cpg	351.75	J/mol×K	727.29	Joback Method
cpg	359.13	J/mol×K	762.80	Joback Method
cpg	365.90	J/mol×K	798.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C339593&Units=SI

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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