3,5-Bis(trifluoromethyl)benzhydrazide

Other names:	3,5-di(Trifluoromethyl)benzhydrazide
	Benzoic acid, 3,5-bis(trifluoromethyl)-, hydrazide
	3,5-Bis(trifluoromethyl)benzoylhydrazine
	3,5-bis(trifluoromethyl)benzohydrazide
Inchi:	InChI=1S/C9H6F6N2O/c10-8(11,12)5-1-4(7(18)17-16)2-6(3-5)9(13,14)15/h1-3H,16H2,(H
InchiKey:	GBBRFBSFWKFTMZ-UHFFFAOYSA-N
Formula:	C9H6F6N2O
SMILES:	NNC(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	272.15
CAS:	26107-82-4

Physical Properties

Property code	Value	Unit	Source
gf	-1018.21	kJ/mol	Joback Method
hf	-1234.98	kJ/mol	Joback Method
hfus	27.88	kJ/mol	Joback Method
hvap	55.56	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	2.328		Crippen Method
mcvol	146.060	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	607.69	K	Joback Method
tc	802.06	K	Joback Method
tf	436.88	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.45	J/mol×K	607.69	Joback Method
cpg	398.26	J/mol×K	640.09	Joback Method
cpg	407.29	J/mol×K	672.48	Joback Method
cpg	415.58	J/mol×K	704.88	Joback Method
cpg	423.18	J/mol×K	737.27	Joback Method

cpg	430.16	J/mol×K	769.67	Joback Method
cpg	436.56	J/mol×K	802.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26107824&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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