3-(Trifluoromethyl)benzyl mercaptan

Other names: 3-Trifluoromethylbenzyl mercaptan
3-Trifluoromethyl benzylthiol
Inchi: InChI=1S/C8H7F3S/c9-8(10,11)7-3-1-2-6(4-7)5-12/h1-4,12H,5H2
InchiKey: CQIQWIMXCPTQPJ-UHFFFAOYSA-N
Formula: C8H7F3S
SMILES: FC(F)(F)c1cccc(CS)c1
Mol. weight [g/mol]: 192.21

Physical Properties

Property code	Value	Unit	Source
hf	-595.76	kJ/mol	Cheméo Relay (1.0)
hfus	16.00	kJ/mol	Joback Method
hvap	55.51	kJ/mol	Cheméo Relay (1.0)
ie	9.32	eV	Cheméo Relay (1.0)
log10ws	-2.37		Cheméo Relay (1.0)
logp	3.135		Crippen Method
mcvol	121.480	ml/mol	McGowan Method
tb	456.42	K	Cheméo Relay (1.0)
tc	674.15	K	Cheméo Relay (1.0)
tf	260.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.62	J/mol×K	471.54	Joback Method
cpg	261.63	J/mol×K	507.20	Joback Method
cpg	272.75	J/mol×K	542.87	Joback Method
cpg	283.04	J/mol×K	578.53	Joback Method
cpg	292.55	J/mol×K	614.20	Joback Method
cpg	301.32	J/mol×K	649.86	Joback Method
cpg	309.41	J/mol×K	685.52	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25697556&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point