Benzodiazepine, 1h-1,4-, 2,3-dihydro-5-phenyl-7-(trifluoromethyl)-

Inchi: InChI=1S/C16H13F3N2/c17-16(18,19)12-6-7-14-13(10-12)15(21-9-8-20-14)11-4-2-1-3-5-

InchiKey: UVIWKJUMUWEHQO-UHFFFAOYSA-N

Formula: C16H13F3N2

SMILES: FC(F)(F)c1ccc2c(c1)C(c1ccccc1)=NCCN2

Mol. weight [g/mol]: 290.28

CAS: 2890-28-0

Physical Properties

Property code	Value	Unit	Source
gf	-23.11	kJ/mol	Joback Method
hf	-284.62	kJ/mol	Joback Method
hfus	34.75	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.968		Crippen Method
mcvol	198.890	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	749.72	K	Joback Method
tc	1003.42	K	Joback Method
tf	557.14	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.54	J/mol×K	749.72	Joback Method
cpg	593.70	J/mol×K	792.00	Joback Method
cpg	608.31	J/mol×K	834.29	Joback Method
cpg	621.47	J/mol×K	876.57	Joback Method
cpg	633.27	J/mol×K	918.85	Joback Method
cpg	643.82	J/mol×K	961.14	Joback Method
cpg	653.21	J/mol×K	1003.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2890280&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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