

Clobenzorex, N-trifluoroacetyl

Other names:	Clobenzorex N-TFA Chlorbenzorex N-TFA
Inchi:	InChI=1S/C18H17ClF3NO/c1-13(11-14-7-3-2-4-8-14)23(17(24)18(20,21)22)12-15-9-5-6-
InchiKey:	PDNDDUSCICVEBH-UHFFFAOYSA-N
Formula:	C18H17ClF3NO
SMILES:	CC(Cc1ccccc1)N(Cc1ccccc1Cl)C(=O)C(F)(F)F
Mol. weight [g/mol]:	355.78

Physical Properties

Property code	Value	Unit	Source
gf	-298.23	kJ/mol	Joback Method
hf	-616.41	kJ/mol	Joback Method
hfus	37.19	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.862		Crippen Method
mcvol	246.060	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
tb	767.46	K	Joback Method
tc	984.04	K	Joback Method
tf	459.49	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.22	J/molxK	767.46	Joback Method
cpg	705.57	J/molxK	803.56	Joback Method
cpg	718.79	J/molxK	839.65	Joback Method
cpg	730.97	J/molxK	875.75	Joback Method
cpg	742.22	J/molxK	911.85	Joback Method
cpg	752.65	J/molxK	947.95	Joback Method
cpg	762.34	J/molxK	984.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292767&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
hvp:	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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