Clobenzorex, AC

Inchi: InChI=1S/C18H20ClNO/c1-14(12-16-8-4-3-5-9-16)20(15(2)21)13-17-10-6-7-11-18(17)19
InchiKey: KRTYUJXALHAFCT-UHFFFAOYSA-N
Formula: C18H20ClNO
SMILES: CC(=O)N(Cc1ccccc1Cl)C(C)Cc1ccccc1
Mol. weight [g/mol]: 301.81

Physical Properties

Property code	Value	Unit	Source
gf	283.36	kJ/mol	Joback Method
hf	-19.33	kJ/mol	Joback Method
hfus	35.36	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.320		Crippen Method
mcvol	240.750	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
tb	772.88	K	Joback Method
tc	1004.68	K	Joback Method
tf	455.30	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.14	J/mol×K	772.88	Joback Method
cpg	682.11	J/mol×K	811.51	Joback Method
cpg	696.83	J/mol×K	850.15	Joback Method
cpg	710.38	J/mol×K	888.78	Joback Method
cpg	722.86	J/mol×K	927.41	Joback Method
cpg	734.36	J/mol×K	966.04	Joback Method
cpg	744.97	J/mol×K	1004.68	Joback Method

Sources

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=R269413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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