Norfluoxetine

Other names: 3-Phenyl-3-[4-(trifluoromethyl)phenoxy]-1-propanamine
Inchi: InChI=1S/C16H16F3NO/c17-16(18,19)13-6-8-14(9-7-13)21-15(10-11-20)12-4-2-1-3-5-12
InchiKey: WIQRCHMSJFFONW-UHFFFAOYSA-N
Formula: C16H16F3NO
SMILES: NCCC(Oc1ccc(C(F)(F)F)cc1)c1ccccc1
Mol. weight [g/mol]: 295.30
CAS: 56161-73-0

Physical Properties

Property code	Value	Unit	Source
gf	-323.55	kJ/mol	Joback Method
hf	-612.77	kJ/mol	Joback Method
hfus	29.58	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.174		Crippen Method
mcvol	209.940	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1868.10		NIST Webbook
tb	712.91	K	Joback Method
tc	933.52	K	Joback Method
tf	430.12	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.52	J/mol×K	712.91	Joback Method
cpg	606.69	J/mol×K	749.68	Joback Method
cpg	620.68	J/mol×K	786.45	Joback Method
cpg	633.56	J/mol×K	823.22	Joback Method
cpg	645.40	J/mol×K	859.99	Joback Method
cpg	656.29	J/mol×K	896.76	Joback Method
cpg	666.30	J/mol×K	933.52	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=C56161730&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume