Fenproporex

Other names: Propanenitrile, 3-[(1-methyl-2-phenylethyl)amino]-, (.+/-.)-
Propionitrile, 3-((«alpha»-methylphenethyl)amino)-, (.+/-.)-
(.+/-.)-3-[(«alpha»-Methylphenethyl)amino]propionitrile
N-(2-Cyanoethyl)amphetamine
(.+/-.)-N-2-Cyanoethylamphetamine

Inchi: InChI=1S/C12H16N2/c1-11(14-9-5-8-13)10-12-6-3-2-4-7-12/h2-4,6-7,11,14H,5,9-10H2,1

InchiKey: IQUFSXIQAFPIMR-UHFFFAOYSA-N

Formula: C12H16N2

SMILES: CC(Cc1ccccc1)NCCC#N

Mol. weight [g/mol]: 188.27

CAS: 15686-61-0

Physical Properties

Property code	Value	Unit	Source
gf	382.70	kJ/mol	Joback Method
hf	158.59	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	61.11	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.121		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
tb	652.45	K	Joback Method
tc	871.40	K	Joback Method
tf	354.07	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.78	J/mol×K	652.45	Joback Method
cpg	446.85	J/mol×K	688.94	Joback Method
cpg	459.98	J/mol×K	725.43	Joback Method
cpg	472.23	J/mol×K	761.93	Joback Method

cpg	483.65	J/mol×K	798.42	Joback Method
cpg	494.28	J/mol×K	834.91	Joback Method
cpg	504.17	J/mol×K	871.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15686610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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