MEFENOREX

Other names: Phenethylamine, N-(3-chloropropyl)-«alpha»-methyl-
Mefenorex
N-(3-Chloropropyl)-«alpha»-methylphenethylamine
Inchi: InChI=1S/C12H18ClN/c1-11(14-9-5-8-13)10-12-6-3-2-4-7-12/h2-4,6-7,11,14H,5,8-10H2,1
InchiKey: XXVROGAVTTXONC-UHFFFAOYSA-N
Formula: C12H18ClN
SMILES: CC(Cc1ccccc1)NCCCCl
Mol. weight [g/mol]: 211.74

Physical Properties

Property code	Value	Unit	Source
af	0.5189		Cheméo Relay (1.0)
hf	-46.03	kJ/mol	Cheméo Relay (1.0)
hfus	26.65	kJ/mol	Joback Method
hvap	72.97	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-1.50		Cheméo Relay (1.0)
logp	2.836		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
tb	557.69	K	Cheméo Relay (1.0)
tc	766.41	K	Cheméo Relay (1.0)
tf	285.47	K	Cheméo Relay (1.0)
vc	0.621	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.00	J/mol×K	587.80	Joback Method
cpg	445.05	J/mol×K	622.62	Joback Method
cpg	460.12	J/mol×K	657.43	Joback Method
cpg	474.25	J/mol×K	692.25	Joback Method
cpg	487.50	J/mol×K	727.07	Joback Method
cpg	499.90	J/mol×K	761.89	Joback Method

cpg	511.50	J/mol×K	796.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17243571&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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