Fenproporex-M (HO-methoxy-), 2AC

Inchi: InChI=1S/C17H22N2O4/c1-12(19(13(2)20)9-5-8-18)10-15-6-7-16(23-14(3)21)11-17(15)2
InchiKey: YYZUVNKTGDQKDF-UHFFFAOYSA-N
Formula: C17H22N2O4
SMILES: COc1cc(OC(C)=O)ccc1CC(C)N(CCC#N)C(C)=O
Mol. weight [g/mol]: 318.37

Physical Properties

Property code	Value	Unit	Source
gf	-40.91	kJ/mol	Joback Method
hf	-443.09	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	87.48	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.314		Crippen Method
mcvol	252.870	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
tb	891.66	K	Joback Method
tc	1107.88	K	Joback Method
tf	559.59	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.16	J/mol×K	891.66	Joback Method
cpg	780.48	J/mol×K	927.70	Joback Method
cpg	791.68	J/mol×K	963.73	Joback Method
cpg	801.79	J/mol×K	999.77	Joback Method
cpg	810.82	J/mol×K	1035.80	Joback Method
cpg	818.80	J/mol×K	1071.84	Joback Method
cpg	825.74	J/mol×K	1107.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R275126&Units=SI

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