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

Inchi: InChI=1S/C14H19NO4/c1-9(15-10(2)16)7-12-5-6-13(19-11(3)17)8-14(12)18-4/h5-6,8-9H

InchiKey: IIKBNVUEUSHLHM-UHFFFAOYSA-N

Formula: C14H19NO4

SMILES: COc1cc(OC(C)=O)ccc1CC(C)NC(C)=O

Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
gf	-220.74	kJ/mol	Joback Method
hf	-560.11	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	1.688		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2065.00		NIST Webbook
tb	758.67	K	Joback Method
tc	969.08	K	Joback Method
tf	480.98	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.32	J/mol×K	758.67	Joback Method
cpg	607.23	J/mol×K	793.74	Joback Method
cpg	620.16	J/mol×K	828.81	Joback Method
cpg	632.13	J/mol×K	863.87	Joback Method
cpg	643.13	J/mol×K	898.94	Joback Method
cpg	653.17	J/mol×K	934.01	Joback Method
cpg	662.25	J/mol×K	969.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R275151&Units=SI
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

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