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

Inchi: InChI=1S/C16H23NO4/c1-6-17(12(3)18)11(2)9-14-7-8-15(21-13(4)19)10-16(14)20-5/h7-8
InchiKey: ZTOKZGINPRAKCT-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CCN(C(C)=O)C(C)Cc1ccc(OC(C)=O)cc1OC
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
gf	-182.51	kJ/mol	Joback Method
hf	-587.33	kJ/mol	Joback Method
hfus	35.53	kJ/mol	Joback Method
hvap	74.78	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.420		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	766.70	K	Joback Method
tc	970.54	K	Joback Method
tf	483.33	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.83	J/mol×K	766.70	Joback Method
cpg	704.15	J/mol×K	800.67	Joback Method
cpg	718.44	J/mol×K	834.65	Joback Method
cpg	731.71	J/mol×K	868.62	Joback Method
cpg	743.99	J/mol×K	902.59	Joback Method
cpg	755.28	J/mol×K	936.56	Joback Method
cpg	765.60	J/mol×K	970.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R264765&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

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