Ethylamphetamine-M (di-HO-), 3AC

Inchi: InChI=1S/C17H23NO5/c1-6-18(12(3)19)11(2)9-15-7-8-16(22-13(4)20)10-17(15)23-14(5)
InchiKey: PHZSGMXGHURGHA-UHFFFAOYSA-N
Formula: C17H23NO5
SMILES: CCN(C(C)=O)C(C)Cc1ccc(OC(C)=O)cc1OC(C)=O
Mol. weight [g/mol]: 321.37

Physical Properties

Property code	Value	Unit	Source
gf	-303.01	kJ/mol	Joback Method
hf	-720.55	kJ/mol	Joback Method
hfus	39.72	kJ/mol	Joback Method
hvap	83.75	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.337		Crippen Method
mcvol	253.060	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	843.45	K	Joback Method
tc	1053.02	K	Joback Method
tf	544.53	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.26	J/mol×K	843.45	Joback Method
cpg	775.04	J/mol×K	878.38	Joback Method
cpg	787.70	J/mol×K	913.31	Joback Method
cpg	799.26	J/mol×K	948.24	Joback Method
cpg	809.73	J/mol×K	983.16	Joback Method
cpg	819.13	J/mol×K	1018.09	Joback Method
cpg	827.48	J/mol×K	1053.02	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=R264750&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