Isophthalic acid, monoamide, N-(3-methylphenyl)-, ethyl ester

Inchi: InChI=1S/C17H17NO3/c1-3-21-17(20)14-8-5-7-13(11-14)16(19)18-15-9-4-6-12(2)10-15/h
InchiKey: LGSYMCXYGNBWMV-UHFFFAOYSA-N
Formula: C17H17NO3
SMILES: CCOC(=O)c1cccc(C(=O)Nc2cccc(C)c2)c1
Mol. weight [g/mol]: 283.32

Physical Properties

Property code	Value	Unit	Source
gf	24.37	kJ/mol	Joback Method
hf	-248.00	kJ/mol	Joback Method
hfus	36.57	kJ/mol	Joback Method
hvap	81.65	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.424		Crippen Method
mcvol	221.860	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2649.00		NIST Webbook
rinpol	2649.00		NIST Webbook
tb	832.01	K	Joback Method
tc	1065.87	K	Joback Method
tf	533.98	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.87	J/mol×K	832.01	Joback Method
cpg	651.09	J/mol×K	870.99	Joback Method
cpg	663.14	J/mol×K	909.96	Joback Method
cpg	674.04	J/mol×K	948.94	Joback Method
cpg	683.84	J/mol×K	987.92	Joback Method
cpg	692.61	J/mol×K	1026.89	Joback Method
cpg	700.37	J/mol×K	1065.87	Joback Method

Sources

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=U345785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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