Isophthalic acid, monoamide, N,N-diisobutyl-, ethyl ester

Other names: Isophthalic acid, monoamide, N-diisobutyl-, ethyl ester
Inchi: InChI=1S/C18H27NO3/c1-6-22-18(21)16-9-7-8-15(10-16)17(20)19(11-13(2)3)12-14(4)5/h
InchiKey: WJUFSUUEQIXODL-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CCOC(=O)c1cccc(C(=O)N(CC(C)C)CC(C)C)c1
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-53.48	kJ/mol	Joback Method
hf	-490.20	kJ/mol	Joback Method
hfus	36.39	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.617		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	784.62	K	Joback Method
tc	988.33	K	Joback Method
tf	456.12	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.91	J/mol×K	784.62	Joback Method
cpg	791.45	J/mol×K	818.57	Joback Method
cpg	806.88	J/mol×K	852.52	Joback Method
cpg	821.25	J/mol×K	886.48	Joback Method
cpg	834.59	J/mol×K	920.43	Joback Method
cpg	846.94	J/mol×K	954.38	Joback Method
cpg	858.34	J/mol×K	988.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345794&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